

ANALYTICAL INVESTIGATIONS ON PROPERTIES OF REACTANTS [H₂ - AIR] AND PRODUCTS AT DIFFERENT EQUIVALENCE RATIO

VIKAS J. PATEL¹ & S. A. CHANNIWALA²

¹CK Pithawala College of Engineering and Technology, Surat, Gujarat, India ²Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat, India

ABSTRACT

The rapidly increasing worldwide demand for energy and the progressive depletion of fossil fuels has led to an intensive research for alternative fuels which can be produced on a renewable basis.

Hydrogen in the form of energy will almost certainly be one of the most important energy components of the early next century. Hydrogen is a clean burning and easily transportable fuel. Most of the pollution problems posed by fossil fuels at present would practically disappear with Hydrogen since steam is the main product of its combustion.

The various properties of hydrogen (specific heat, thermal conductivity, kinematic viscosity, density, prandtl no.) have been calculated at various equivalence ratios at different temperatures. Graphs of these properties have been plotted. The software of various property of hydrogen and calculation of all properties was developed using the turbo C language.

KEYWORDS: Computer Simulation, Mathematical Model, Delayed Entry Technique, Hydrogen Fuel

INTRODUCTION

The rapidly increasing worldwide demand for energy and the progressive depletion of fossil fuels has led to an intensive research for alternative fuels which can be produced on a renewable basis.

Hydrogen in the form of energy will almost certainly be one of the most important energy components of the early next century. Hydrogen is a clean burning and easily transportable fuel. Most of the pollution problems posed by fossil fuels at present would practically disappear with Hydrogen since steam is the main product of its combustion.

CRITERIA FOR THE FUTURE FUEL SYSTEM

Many investigations and studies have led to the recognition that the creative scope of a future energy supply is large that there are energy supply options other than mere expansion of conventional energy sources. Discussion for one or the other option therefore has to be carefully prepared. The criteria for future fuel system are listed below:

TECHNOLOGY / ECOLOGY EFFICIENCY

Energy conversion efficiency (Primary energy to usable energy)

Type of primary energy

Raw material requirements, ability o be mined or recycle, possible use of or disposal of water.

Land requirements, effect on climate, ground water etc.

OPERATING EFFICIENCY

Specific energy costs.(at start-up, total lifetime, progressions)

Requisite up-front payments, type of costs.

Amortization times, break-even point etc.

ECONOMIC EFFICIENCY

Influence on economic structures

Effect on employment

Export potential, influence on balance of trade and output

- # Costs of prevention pr repair of ecological or societal damage
- # Repercussions on residential and transportation structures

SUPPLY ASSURANCE

Technical availability under normal operations, life-span etc

Potential dangers and safety in case of accidents

System flexibility under changing conditions (short and medium term, e.g. delivery, restrictions, long term, e.g. substitution of an energy carrier)

SOCIAL COMPATIBILITY

Expansion or restriction of development and room for manoeurve of potential entities, economic entities and the individual; Compatibility with democratic groundless

Compatibility with practice and principles of international trade and with interest of the trading partner

PROPERTIES OF HYDROGEN

Physical Properties

Hydrogen is a colorless and odorless gas. Its density is 0.0899 g/l (air is 14.4 times as dense). Hydrogen boils at -252.77°C. Liquid hydrogen has a density of 70.99 g/l. With these properties, hydrogen has the highest energy to weight ratio of all fuels. 1 kg of hydrogen contains the same amount of energy as 2.1 kg of natural gas or 2.8 kg of gasoline. The energy to volume ratio amounts to about 1/4 of that for petroleum and 1/3 of that for natural gas. Water consists of 11.2% hydrogen by weight. Hydrogen burns in air at concentrations in the range of 4 - 75% by volume (methane burns at 5.3 - 15% and propane at 2.1 - 9.5% concentrations by volume). The highest burning temperature of hydrogen of 2318 °C is reached at 29% concentration by volume, whereas hydrogen in an oxygen atmosphere can reach burning temperatures up to 3000°C (the highest reached burning temperature in air for methane is 2148°C and for propane 2385°C). The minimum required ignition energy required for a stoichiometric fuel/oxygen mixture is for hydrogen 0.02 mJ, for methane 0.29 mJ and for propane 0.26 mJ. Even the energy of a static electric discharge from the arcing of a spark is sufficient to ignite natural gas so it is largely irrelevant that hydrogen requires only a tenth of this energy for ignition. The temperatures for spontaneous combustion of hydrogen, methane and propane are 585°C, 540°C and 487°C respectively.

The explosive regions for hydrogen and methane lie in the ranges 13% - 59% and 6.3% - 14% respectively. The explosive range for hydrogen is clearly much greater, whereas methane is already explosive at a much lower concentration. The diffusion coefficient for hydrogen at 0.61 cm3/s is 4 times as high as that for methane. Hydrogen therefore mixes in air considerably faster than methane or petrol vapor, which is advantageous in the open but represents a potential disadvantage in badly ventilated interiors. Since both hydrogen and natural gas are lighter than air they rise quickly. Propane and petrol vapor are in contrast heavier than air and remain on the ground, leading to a higher likelihood of explosion.

ENVIRONMENTAL ADVANTAGES

The burning of hydrogen with air under appropriate conditions in combustion engines or gas turbines results in very low or negligible emissions. Trace hydrocarbon and carbon monoxide emissions, if at all generated, can only result from the combustion of motor oil in the combustion chamber of internal combustion engines. Nitrous oxide emissions increase exponentially with the combustion temperature. These can therefore be influenced through appropriate process control. As hydrogen offers more possibilities than other fuels, a distinct reduction in NOx emissions is possible compared to mineral oil and natural gas, provided that a lower combustion temperature is achieved (e.g. with a high air to fuel ratio). Particulate and sulfur emissions are completely avoided apart from small quantities of lubricant remnants.

The use of hydrogen in fuel cell propulsion systems with low temperature fuel cells (Membrane fuel cells: PEMFC) completely eliminates all polluting emissions. The only by-product resulting from the generation of electricity from hydrogen and oxygen in the air is de-mineralised water. Use of hydrogen in fuel cells at higher temperature levels causes up to 100 times fewer emissions compared with conventional power stations. If the hydrogen is obtained from methanol however, then the reforming process itself will result in carbon dioxide emissions.

Furthermore hydrogen offers the possibility, depending on production method, to drastically reduce or avoid emissions, especially carbon dioxide (CO2), in the whole fuel cycle. Using hydrogen as secondary energy carrier would allow the flexible introduction of the most diverse renewable energies into the fuel sector.

Since hydrogen is a secondary energy carrier, the complete fuel cycle from primary energy source to final application must be considered when judging the environmental relevance.

COMPOUNDS

Although pure Hydrogen is a gas we find very little of it in our atmosphere. Hydrogen gas is so light that uncombined Hydrogen will gain enough velocity from collisions with other gases that they will quickly be ejected from the atmosphere. On earth, hydrogen occurs chiefly in combination with oxygen in water, but it is also present in organic matter such as living plants, petroleum, coal, etc. It is present as the free element in the atmosphere, but only to the extent of less than 1 ppm by volume. The lightest of all gases, hydrogen combines with other elements – sometimes explosively -- to form compounds.

FORMS

Quite apart from isotopes, it has been shown that under ordinary conditions hydrogen gas is a mixture of two kinds of molecules, known as ortho- and para-hydrogen, which differ from one another by the spins of their electrons and nuclei.

Normal hydrogen at room temperature contains 25% of the para form and 75% of the ortho form. The ortho form cannot be prepared in the pure state. Since the two forms differ in energy, the physical properties also differ. The melting and boiling points of parahydrogen are about 0.1oC lower than those of normal hydrogen.

ISOTOPES

The ordinary isotope of hydrogen, H, is known as Protium, the other two isotopes are Deuterium (a proton and a neutron) and Tritium (a protron and two neutrons). Hydrogen is the only element whose isotopes have been given different names. Deuterium and Tritium are both used as fuel in nuclear fusion reactors. One atom of Deuterium is found in about 6000 ordinary hydrogen atoms.

Deuterium is used as a moderator to slow down neutrons. Tritium atoms are also present but in much smaller proportions. Tritium is readily produced in nuclear reactors and is used in the production of the hydrogen (fusion) bomb. It is also used as a radioactive agent in making luminous paints, and as a tracer.

GENERAL STRUCTURE

Atomic Number: 1

Group: 1

Period: 1

Series: Nonmetals

NAME IN OTHER LANGUAGES

- Latin: Hydrogenium
- Czech: Vodík
- Croatian: Vodik
- French: Hydrogéne
- German: Wasserstoft r
- Italian: Idrogeno
- Norwegian: Hydrogen
- Portuguese: Hidrogênio
- Spanish: Hidrógeno
- Swedish: Väte

ATOMIC STRUCTURE

- Atomic Radius: 0.79Å
- Atomic Volume: 14.4cm3/mol

- Covalent Radius: 0.32Å
- Cross Section: 0.33barns
- Crystal Structure: Hexagonal
- Electron Configuration: 1s1
- Electrons per Energy Level: 1

SHELL MODEL

- Ionic Radius: 0.012Å
- Filling Orbital: 1s1
- Number of Electrons (with no charge): 1
- Number of Neutrons (most common/stable nuclide): 0
- Number of Protons: 1
- Oxidation States: 1
- Valance Electrons: 1s1

CHEMICAL PROPERTIES

- Electrochemical Equivalent: 0.037605g/amp-hr
- Electron Work Function:
- Electronegativity (Pauling): 2.2
- Heat of Fusion: 0.05868kJ/mol
- Incompatibilities: metals, oxidizing materials, metal oxides, combustible materials, halogens, metal salts, halo carbons
- Ionization Potential First: 13.598
- Valance Electron Potential (-eV): 1200

REGULATORY / HEALTH

- CAS Number
- 1333-74-0 Compressed gas
- UN/NA ID and ERG Guide Number
- UN1049 / 115 Compressed gasUN1966 / 115 Refrigerated liquid
- RTECS: MW8900000
- NFPA 704

Health: 1

Fire: 4

Reactivity: 0

Special Hazard:

• OSHA Permissible Exposure Limit (PEL)

No limits set by OSHA

• OSHA PEL Vacated 1989

No limits set by OSHA

• NIOSH Recommended Exposure Limit (REL)

No limits set by NIOSH

COMBUSTION OF HYDROGEN

• Hydrogen burns in oxygen or air to form water.

2 H2 + O2 ==> 2 H2O

- Oxygen will also burn in hydrogen.
- Hydrogen does not itself support combustion, as may be shown by passing a lighted taper into an inverted jar of hydrogen, when the taper is extinguished.

A mixture of hydrogen with oxygen or air explodes violently when kindled, provided either gas is not present in too large excess.

REACTION STOICHIOMETRY AND COMPUTATION OF MASS FRACTION AND PROPERTIES OF REACTANTS AND PRODUCTS

Stoichiometric Reaction for ($\phi < 1$)

$$H_{2} + \frac{1}{2\phi} [O_{2} + 3.762N_{2}] \rightarrow (H_{2}O)_{g} + \frac{1}{2} (\frac{1-\phi}{\phi})O_{2} + (\frac{1.881}{\phi})N_{2}$$

Mass Fractions of Reactants

Total mass of reactants m_r :

$$m_r = 2 + \left(\frac{1}{2\phi} \times 137.336\right) kg$$
$$= 2\left(\frac{\phi + 34.334}{\phi}\right) kg$$

Mass fraction of H₂; $X_{H_2,r}$

$$X_{H_2,r} = \frac{2}{m_r}$$

Mass fraction of O₂; $X_{O_2,r}$

$$X_{O_2,r} = \frac{16}{m_r \times \phi}$$

Mass fraction of N₂; $X_{N_2,r}$

$$X_{N_2,r} = \frac{52.668}{m_r \times \phi}$$

Mass Fraction of Products

Total mass of Products: m_p

$$m_p = 18 + (16)\left(\frac{1-\phi}{\phi}\right) + \frac{52.668}{\phi}kg$$

Mass fraction of H₂O; $X_{H_2O,p}$

$$X_{H_2O,p} = \frac{18}{m_p}$$

Mass fraction of O₂; $X_{O_2,p}$

$$X_{O_2,p} = \frac{16\left(\frac{1-\phi}{\phi}\right)}{m_p}$$

Mass fraction of N₂; $X_{N_2,p}$

$$X_{N_2,p} = \frac{52.668}{m_p \times \phi}$$

Stoichiometric Reaction for ($\phi = 1$)

$$H_2 + \frac{1}{2} [O_2 + 3.762N_2] \rightarrow H_2O_g + 1.881N_2$$

Mass Fractions of Reactants

Total mass of reactants m_r

www.iaset.us

$$m_r = 2 + \left(\frac{1}{2}\phi \times 137.336\right) kg$$
$$= 70.668 kg$$

Mass fraction of H₂; $X_{H_2,r}$

$$X_{H_2,r} = \frac{2}{70.668} = 0.0283$$

Mass fraction of O₂; $X_{O_2,r}$

$$X_{O_2,r} = \frac{16}{70.668} = 0.2264$$

Mass fraction of N₂; $X_{N_2,r}$

$$X_{N_2,r} = \frac{52.668}{70.668} = 0.7453$$

Mass Fraction of Products

Total mass of Products: m_p

$$m_p = 18 + (16)\left(\frac{1-\phi}{\phi}\right) + \frac{52.668}{\phi}kg$$

Mass fraction of H₂O; $X_{H_2O,p}$

$$X_{H_2O,p} = \frac{18}{m_p} = \frac{18}{70.668} = 0.2547$$

Mass fraction of O₂; $X_{O_2,r}$

$$X_{O_2,p} = \frac{16\left(\frac{1-\phi}{\phi}\right)}{m_p} = 0$$

Mass fraction of N₂; $X_{N_2, p}$

$$X_{N_{2,p}} = \frac{52.668}{70.668} = 0.7453$$

Stoichiometric Reaction for ($\phi > 1$)

$$\phi H_2 + \frac{1}{2} [O_2 + 3.762N_2] \rightarrow (H_2O)_g + (\phi - 1)H_2 + 1.881N_2$$

Mass Fractions of Reactants

Total mass of reactants m_r

$$m_r = 2\phi + 68.668 \, kg$$

Mass fraction of H₂; $X_{H_2,r}$

$$X_{H_2,r} = \frac{2\phi}{m_r}$$

Mass fraction of O₂; $X_{O_2,r}$

$$X_{O_2,r} = \frac{16}{m_r}$$

Mass fraction of N₂; $X_{N_2,r}$

$$X_{N_2,r} = \frac{52.668}{m_r}$$

Mass Fraction of Products

Total mass of Products: m_p

$$m_p = 18 + 2 \times (\phi - 1) + 52.668 \ kg$$

Mass fraction of H₂O; $X_{H_2O,p}$

$$X_{H_2O,p} = \frac{18}{m_p}$$

Mass fraction of H₂; $X_{H_2,p}$

$$X_{H_2,p} = \frac{2(\phi - 1)}{m_p}$$

Mass fraction of N₂; $X_{N_2,p}$

$$X_{N_2,p} = \frac{52.668}{m_p}$$

Specific Heat of Reactants

$$C_{p_r,T_r} = X_{H_2,r} C_{p_{H_2,T_r}} + X_{O_2,r} C_{p_{O_2,T_r}} + X_{N_2,r} C_{p_{N_2,T_r}}$$

Specific Heat of Products

$$C_{p_{p},T_{p}} = X_{H_{2},p}C_{p_{H_{2},T_{p}}} + X_{O_{2},p}C_{p_{O_{2},T_{p}}} + X_{N_{2},p}C_{p_{N_{2},T_{p}}} + X_{H_{2}O,p}C_{p_{H_{2}O,T_{p}}}$$

Thermal Conductivity for Reactants

$$K_{r,T_r} = X_{H_2,r} K_{H_2,T_r} + X_{O_2,r} K_{O_2,T_r} + X_{N_2,r} K_{N_2,T_r}$$

Thermal Conductivity for Products

$$K_{p,T_p} = X_{H_2O,p} K_{H_2O,T_p} + X_{O_2,p} K_{O_2,T_p} + X_{N_2,p} K_{N_2,T_p} + X_{H_2,p} K_{H_2,T_p}$$

Density for Reactants

$$\rho_{r,T_r} = X_{H_2,r} \rho_{H_2,T_r} + X_{O_2,r} \rho_{O_2,T_r} + X_{N_2,r} \rho_{N_2,T_r}$$

Density for Products

$$\rho_{p,T_p} = X_{H_2O,p} \rho_{H_2O,T_p} + X_{O_2,p} \rho_{O_2,T_p} + X_{N_2,p} \rho_{N_2,T_p} + X_{H_2,p} \rho_{H_2,T_p}$$

Molecular Mass for Reactants

$$M_{eq,r} = X_{H_2,r} M_{H_2} + X_{O_2,r} M_{O_2} + X_{N_2,r} M_{N_2}$$

Gas Constant for Reactants

$$R_{eq,r} = \frac{R}{M_{eq,r}}$$

Molecular Mass for Products

$$M_{eq,p} = X_{H_2O,p}M_{H_2O} + X_{O_2,p}M_{O_2} + X_{N_2,p}M_{N_2} + X_{H_2,p}M_{H_2}$$

Gas Constant for Products

$$R_{eq,p} = \frac{R}{M_{eq,p}}$$

Specific Heat at Constant Volume for Reactants

$$C_{v_r,T_r} = R_{eq,r} - C_{p_r,T_r}$$

Specific Heat at Constant Volume for Products

$$C_{v_p,T_p} = R_{eq,p} - C_{p_p,T_p}$$

Specific Heat Ratio for Reactants

$$\gamma_{r,T_r} = \frac{C_{p_r,T_r}}{C_{v_r,T_r}}$$

57

Specific Heat Ratio for Products

$$\gamma_{p,T_p} = \frac{C_{p_p,T_p}}{C_{v_p,T_p}}$$

RESULTS & DISCUSSIONS

Results obtained using above analysis are given in Appendix 1 and graphs are plotted accordingly.

CONCLUSIONS

Usually Hydrogen-air engine are operated in a equivalence ratio range of 0.6 to 1.0 [1, 2] and hence all the physical properties of reactants and products are evaluated in the wider equivalence ratio range of 0.2 to 1.4 for simulation purpose.

The typical variations of specific heats only for reactants and products in the equivalence ratio range of 0.2 to 1.4 are depicted in Figure 1 to Figure 10, respectively as a function of temperature. The individual constituent properties are taken from Roshenow et. al. [61]. These properties of reactants and products are used as input parameters for digital simulation of Hydrogen-air engine.

REFFRENCES

- 1. Heywood J.B. "Internal Combustion Engine Fundamentals", New York, Mcgrow Hill Book Company, 1988
- 2. Benson Ronald S : "Thermodynamics and Gas Dynamics of Internal Combustion Engine", Oxford University Press Vol. II 1986
- 3. Ganeshan V. "Computer Simulation of S.I.Engine Process, Mcgrow Hill Book Company Hyderabad, 1988
- 4. Richard Stone : "Introduction of I.C. Engine", Macmillan, Volume 1,1989
- President's Council of Advisors on Science and Technology (PCAST) : "Federal Energy Research and Development for the Challenges of the Twenty-First Century", Report of the Energy Research and Development Panel, 5 November., 1997
- Thomas, C.E., James, B.D., & Lomax, F.D. Jr.: "Market Penetration Scenarios for Fuel Cell Vehicles," Procs. 8th Ann. U.S. Hydrogen Mtg., Arlington VA, National Hydrogen Association, 11–13 March; Directed Technologies, Inc. (Arlington, VA 22203, 703/243-3383, fax -2724)., 1997
- 7. Thomas, C.E., Kuhn, I.F. Jr., James, B.D., Lomax, F.D. Jr., & Baum, G.N. : "Affordable Hydrogen Supply Pathways for Fuel Cell Vehicles," Int. J. Hydrogen Energy 23(6):507–516, June., 1998
- Thomas, C.E., James, B.D., Lomax, F.D. Jr., & Kuhn, I.F. Jr. : "Fuel Options for the Fuel Cell Vehicle: Hydrogen, Methanol or Gasoline?," Fuel Cell Reformer Conference, Diamond Bar CA, South Coast Air Quality Management District, 20 November., 1998
- Lovins, A.B.: "Putting Central Power Plants Out of Business," address to Aspen Institute Energy Forum, 7 July, RMI Publication, http://redtail.stanford.edu/seminar/presentations/lovins1/sld001.htm., 1998

- 10. Bauen, A and Hart, D : "Further assessment of the environmental characteristics of fuel cells and competing technologies ETSU Report "F/02/00153/REP, ETSU, Harwell, UK., 1998
- 11. Cole, J: "Interannual-decadal variability in the tropical ocean atmosphere and the extra-tropical response", presentation at the International Conference on Paleoceanography, Lisbon, Aug 24-28.
- 12. Directed Technologies, Inc.: "Integrated analysis of hydrogen passenger vehicle transportation pathways", draft final report for National Renewable Energy Laboratory, US Department of Energy., 1998
- Ekdunge, P and Råberg, M : "The fuel cell vehicle analysis of energy use, emissions and cost", Int J. Hydrogen Energy, Vol. 23, No. 5, pp. 381-385, 1998

APPENDICES

Properties of Reactantas & Products at Different Equvalence Ratios $[\phi = 0.2 \text{ To } 1.4]$

Table 1: Results of Equivalence Ratio $\emptyset = 0.2$ [for Reactants]

equivalence ratio $= 0.2$ for reactant							
The coef	The coeff. of nitrogen is $= 9.404762$						
The total	mass of read	ctants is $= 34$	45.333344				
The mass	s fraction of	hydrogen is	= 0.005792				
The mass	s fraction of	oxygen is =	0.231660				
The mass	s fraction of	nitrogen is =	0.762548				
Temp	Sp.Heat	Cond.	Density	Vis.*10-6	Prandtl No.		
-128.9	1.087693	0.014172	2.446491	4.301892	0.754106		
-17.8	1.086853	0.023729	1.38333	13.90143	0.728573		
93.4	1.09388	0.031227	0.962008	22.99353	0.717597		
204.4	1.110434	0.03854	0.740984	36.11834	0.715276		
315.6	1.133793	0.045657	0.598794	51.69798	0.715873		
426.7	1.159739	0.051981	0.497406	68.61603	0.716913		
537.8	1.187114	0.058208	0.435318	86.60126	0.721952		
538.9	1.213098	0.063597	0.370308	111.0352	0.734008		
760	1.239083	0.068365	0.342097	128.4653	0.745295		

Table 2: Results of Equivalence Ratio $\emptyset = 0.2$ [for Products]

equivalence ratio = 0.2 for product								
Enter ch	Enter choice= 1 for equivalence ratio = 1							
and 2 for	and 2 for eq. ratio > 1 and 3 for eq. ratio $< 1 = 3$							
The coef	ff. of nitrogen	is = 9.405000						
The total	l mass of proc	lucts is $= 345.33$	9996					
The mas	s fraction of v	water is $= 0.0521$	23					
The mas	s fraction of o	oxygen is $= 0.185$	5325					
The mas	s fraction of 1	nitrogen is $= 0.76$	52553					
Temp	Sp.Heat	Cond.*10-3	Density	Vis.*10-6	Prandtl No.			
100	1.072055	21 271567	0.024250	22 40000	0.700.42.6			
100	1.072855	31.3/156/	0.924259	22.48089	0.700436			
200	1.072855	31.3/156/ 38.645306	0.924259	22.48089 33.62896	0.700436			
200 300	1.072855 1.076804 1.097287	31.371567 38.645306 45.435432	0.924259 0.728589 0.60165	22.48089 33.62896 46.55	0.700436 0.674324 0.669895			
200 300 400	1.072855 1.076804 1.097287 1.121009	31.3/1567 38.645306 45.435432 51.779495	0.924259 0.728589 0.60165 0.511857	22.48089 33.62896 46.55 61.23127	0.700436 0.674324 0.669895 0.674527			
200 300 400 500	1.072855 1.076804 1.097287 1.121009 1.147937	31.3/156/ 38.645306 45.435432 51.779495 57.53101	0.924259 0.728589 0.60165 0.511857 0.445255	22.48089 33.62896 46.55 61.23127 77.49941	0.700436 0.674324 0.669895 0.674527 0.676471			
100 200 300 400 500 600	1.072855 1.076804 1.097287 1.121009 1.147937 1.174594	31.371567 38.645306 45.435432 51.779495 57.53101 62.789375	0.924259 0.728589 0.60165 0.511857 0.445255 0.394896	22.48089 33.62896 46.55 61.23127 77.49941 94.71409	0.700436 0.674324 0.669895 0.674527 0.676471 0.690025			
100 200 300 400 500 600 700	1.072855 1.076804 1.097287 1.121009 1.147937 1.174594 1.197827	31.371567 38.645306 45.435432 51.779495 57.53101 62.789375 67.430435	0.924259 0.728589 0.60165 0.511857 0.445255 0.394896 0.354699	22.48089 33.62896 46.55 61.23127 77.49941 94.71409 114.2104	$\begin{array}{r} 0.700436\\ \hline 0.674324\\ \hline 0.669895\\ \hline 0.674527\\ \hline 0.676471\\ \hline 0.690025\\ \hline 0.710424\\ \end{array}$			
100 200 300 400 500 600 700 800	1.072855 1.076804 1.097287 1.121009 1.147937 1.174594 1.197827 1.216931	31.371567 38.645306 45.435432 51.779495 57.53101 62.789375 67.430435 71.578568	0.924259 0.728589 0.60165 0.511857 0.445255 0.394896 0.354699 0.320398	22.48089 33.62896 46.55 61.23127 77.49941 94.71409 114.2104 134.6563	$\begin{array}{r} 0.700436\\ \hline 0.674324\\ \hline 0.669895\\ \hline 0.674527\\ \hline 0.676471\\ \hline 0.690025\\ \hline 0.710424\\ \hline 0.715849 \end{array}$			
100 200 300 400 500 600 700 800 900	1.072855 1.076804 1.097287 1.121009 1.147937 1.174594 1.197827 1.216931 1.239055	31.371567 38.645306 45.435432 51.779495 57.53101 62.789375 67.430435 71.578568 75.158722	0.924259 0.728589 0.60165 0.511857 0.445255 0.394896 0.354699 0.320398 0.293363	22.48089 33.62896 46.55 61.23127 77.49941 94.71409 114.2104 134.6563 156.3397	$\begin{array}{r} 0.700436\\ \hline 0.674324\\ \hline 0.669895\\ \hline 0.674527\\ \hline 0.676471\\ \hline 0.690025\\ \hline 0.710424\\ \hline 0.715849\\ \hline 0.763378\\ \end{array}$			

equivalence ratio = 0.4 for reactant							
The coef	The coeff. of nitrogen is $= 4.702381$						
The tota	l mass of rea	ctants is = 1	73.666672				
The mas	s fraction of	hydrogen is	= 0.011516				
The mas	s fraction of	oxygen is =	0.230326				
The mas	s fraction of	nitrogen is =	= 0.758157				
Temp	Sp.Heat	Cond.	Density	Vis.*10-6	Prandtl No.		
-128.9	1.153177	0.014639	2.433376	4.462591	0.753846		
-17.8	1.162188	0.024509	1.375911	14.31273	0.728507		
93.4	1.170729	0.032263	0.956854	23.75998	0.717495		
204.4	1.187476	0.039832	0.737013	37.28944	0.71505		
315.6	1.210931	0.047185	0.595587	53.35518	0.715545		
426.7	1.236958	0.053743	0.494737	71.00902	0.716597		
537.8	1.264175	0.060095	0.432983	89.0024	0.721578		
538.9	1.29024	0.065631	0.368328	114.6782	0.733622		
760	1.316305	0.070534	0.340263	132.6499	0.744896		

Table 3: Results of Equivalence Ratio $\emptyset = 0.4$ [for Reactants]

Table 4: Results of Equivalence Ratio $\emptyset = 0.4$ [for Products]

Prandtl No.
0.716563
0.686486
0.681332
0.68484
0.683053
0.694921
0.718219
0.724223
0.767405
0.764686
I

Table 5: Results of Equivalence Ratio $\emptyset = 0.6$ [for Reactants]

equivalence ratio $= 0.6$ for reactant							
The coef	The coeff. of nitrogen is $= 3.134795$						
The total	l mass of reac	tants is = 116	.439857				
The mas	s fraction of h	ydrogen is =	0.017176				
The mas	s fraction of c	oxygen is $= 0$.	229007				
The mas	s fraction of r	itrogen is = 0).753816				
Temp	Sp.Heat	Cond.	Density	Vis.*10-6	Prandtl No.		
-128.9	1.217918	0.0151	2.420411	4.621469	0.75359		
-17.8 1.236669 0.02528 1.368576 14.71936 0.728441							
93.4	1.246708	0.033287	0.951757	24.51774	0.717395		
204.4	1.263645	0.04111	0.733088	38.44728	0.714826		

315.6	1.287194	0.048696	0.592416	54.99361	0.715221
426.7	1.313301	0.055485	0.492097	73.3749	0.716284
537.8	1.340362	0.061961	0.430676	91.37634	0.721208
538.9	1.366507	0.067643	0.366371	118.2799	0.73324
760	1.392652	0.072678	0.338451	136.7871	0.744502

Table 6: Results of Equivalence Ratio $\emptyset = 0.6$ [for Products]

equivalence ratio = 0.6for product						
Enter cl	Enter choice= 1 for equivalence ratio = 1					
and 2 fo	or eq. ratio >	1 and 3 for eq. r	atio < 1 =3			
The tota	al mass of pro	oducts is $= 121.4$	75998			
The ma	ss fraction of	water is $= 0.148$	8177			
The ma	ss fraction of	oxygen is $= 0.0$	87721			
The ma	ss fraction of	nitrogen is $= 0.$	764102			
Temp	Sp.Heat	Cond.*10-3	Density	Vis.*10-6	Prandtl No.	
100	1.188371	30.487631	0.880634	22.18219	0.738269	
200	1.174232	37.942604	0.693657	33.24319	0.699749	
300	1.195071	45.061718	0.572895	46.21164	0.692335	
400	1.222052	51.862167	0.487348	61.0074	0.696114	
500	1.252535	58.181118	0.424027	77.41839	0.702276	
600	1.284	64.152939	0.37608	93.94023	0.71431	
700	1.312142	69.60717	0.337716	114.6845	0.729635	
800	1.336527	74.690254	0.305055	135.5131	0.735051	
900	1.364235	79.217888	0.279274	157.5776	0.782166	
1000	1.38392	83.62941	0.257108	181.6148	0.777519	

Table 7: Results of Equivalence Ratio $\emptyset = 0.8$ [for Reactants]

equivalence ratio= 0.8 for reactant							
The coef	f. of nitroge	n is = 2.351	191				
The total	l mass of rea	ctants is = 8	7.833336				
The mas	s fraction of	hydrogen is	= 0.022770				
The mas	s fraction of	oxygen is =	0.227704				
The mas	s fraction of	nitrogen is =	= 0.749526				
Temp	Femp Sp.Heat Cond. Density Vis.*10-6 Prandtl No.						
-128.9	1.281907	0.015556	2.407596	4.778501	0.753336		
-17.8	1.310285	0.026043	1.361326	15.12127	0.728376		
93.4	1.321803	0.034299	0.94672	25.2667	0.717296		
204.4	1.338928	0.042373	0.729209	39.59165	0.714605		
315.6	1.362571	0.050189	0.589282	56.613	0.714901		
426.7	1.388757	0.057207	0.489489	75.71328	0.715975		
537.8	537.8 1.415664 0.063806 0.428394 93.72267 0.720843						
538.9	1.441888	0.069632	0.364436	121.8398	0.732863		
760	1.468112	0.074797	0.336659	140.8763	0.744112		

Table 8: Results of Equivalence Ratio $\emptyset = 0.8$ [for Products]

equivalence ratio = 0.8 for product
Enter choice= 1 for equivalence ratio = 1
and 2 for eq. ratio > 1 and 3 for eq. ratio $< 1 = 3$
The coeff. of nitrogen is $= 2.351250$
The total mass of products is $= 91.834999$
The mass fraction of water is $= 0.196004$
The mass fraction of oxygen is $= 0.087113$

The ma	ss fraction of				
Temp	Sp.Heat	Cond.*10-3	Density	Vis.*10-6	Prandtl No.
100	1.241089	30.114218	0.865344	22.06226	0.75749
200	1.218902	37.69878	0.681208	33.0991	0.71332
300	1.240782	45.026329	0.562656	46.11035	0.70466
400	1.269579	52.109684	0.478599	60.98711	0.707631
500	1.301831	58.778347	0.416432	77.50761	0.713204
600	1.335499	65.172112	0.369351	93.72288	0.723954
700	1.365796	71.103683	0.331659	115.1125	0.739201
800	1.39286	76.730988	0.299576	136.1796	0.744899
900	1.422963	81.808113	0.274274	158.5299	0.789745
1000	1.445241	86.891747	0.252494	182.9019	0.785424

Table 9: Results of Equivalence Ratio $\emptyset = 1.0$ [for Reactants]

equivalence ratio = 1 for reactant							
The coeff	The coeff. of nitrogen is $= 1.880952$						
The total	mass of read	ctants is $= 70$).666664				
The mass	fraction of	hydrogen is	= 0.028302				
The mass	fraction of	oxygen is =	0.226415				
The mass	fraction of	nitrogen is =	0.745283				
Temp	Sp.Heat	Cond.	Density	Vis.*10-6	Prandtl No.		
-128.9	1.345179	0.016007	2.394925	4.933774	0.753085		
-17.8	1.383075	0.026796	1.354158	15.51868	0.728311		
93.4	1.396057	0.0353	0.94174	26.00727	0.717198		
204.4	1.413368	0.043622	0.725373	40.72321	0.714387		
315.6	1.437104	0.051665	0.586183	58.21425	0.714585		
426.7	1.463368	0.058909	0.486909	78.02548	0.71567		
537.8	37.8 1.490123 0.065629 0.426139 96.04273 0.720481						
538.9	1.516425	0.071598	0.362524	125.3597	0.732491		
760	1.542726	0.076892	0.334888	144.9196	0.743726		

Table 10: Results of Equivalence Ratio $\emptyset = 1.0$ [for Products]

equivalence ratio = 1 for product							
Enter cl	Enter choice= 1 for equivalence ratio = 1						
and 2 for	or eq. ratio >	1 and 3 for eq.	ratio < 1 = 3				
The tota	al mass of pr	oducts is $= 70.6$	67999				
The ma	ss fraction of	f water is $= 0.25$	4712				
The ma	ss fraction of	f nitrogen is $= 0$.	.745288				
Temp	Sp.Heat	Cond.*10-3	Density	Vis.*10-6	Prandtl No		
100	1.314438	29.535793	0.835002	21.86322	0.780394		
200	1.280646	37.208611	0.65703	32.83586	0.728338		
300	1.30225	44.7117	0.542746	45.86511	0.717716		
400	1.332929	52.042145	0.461642	60.79812	0.720386		
500	1.367354	59.019184	0.401755	77.38396	0.730074		
600	1.40407	65.810844	0.35634	93.1538	0.740197		
700	1.437532	72.19796	0.319906	115.2924	0.750942		
800	1.467796	78.351677	0.288963	136.566	0.756471		
900	1.501532	83.963417	0.26451	159.0942	0.802245		
1000	1.528286	89.757217	0.243548	183.8772	0.797028		

equivale	equivalence ratio = 1.2 for reactant							
The coe	ff. of nitroge	en is $= 1.880$	952					
The tota	l mass of rea	actants is = 7	71.066666					
The mas	ss fraction of	hydrogen i	s = 0.033771	l				
The mas	ss fraction of	oxygen is =	= 0.225141					
The mas	ss fraction of	f nitrogen is	= 0.741088					
Temp	Cond.	Cond. Sp.Heat Density Vis.*10-6 Prandtl No.						
-128.9	1.407739	0.016452	2.382396	5.087298	0.752837			
-17.8	1.455047 0.027541 1.34707 15.91161 0.728248							
93.4	1.469475 0.036289 0.936815 26.73949 0.717101							
204.4	1.48697 0.044856 0.72158 41.84203 0.714171							
315.6	315.6 1.510797 0.053125 0.583119 59.79747 0.714272							
426.7	1.537139 0.060593 0.484359 80.31164 0.715368							
537.8	1.563743 0.067432 0.423908 98.33669 0.720124							
538.9	1.590122 0.073542 0.360632 128.8401 0.732122							
760	1.616501 0.078964 0.333136 148.9175 0.743345							

Table 11: Results of Equivalence Ratio $\emptyset = 1.2$ [for Reactants]

Table 12: Results of Equivalence Ratio $\emptyset = 1.2$ [for Products]

equivalence ratio = 1.2 for product								
Enter cl	Enter choice= 1 for equivalence ratio = 1							
and 2 fo	or eq. ratio >	1 and 3 for eq.	ratio $< 1 = 3$					
The coe	The coeff. of nitrogen is $= 1.881000$							
The tota	al mass of pr	oducts is $= 71.0$	68001					
The ma	ss fraction o	f water is $= 0.25$	53279					
The ma	ss fraction o	f hydrogen is =	0.005628					
The ma	The mass fraction of nitrogen is $= 0.741093$							
Temp	Sp.Heat	Sp.Heat Cond.*10-3 Density Vis.*10-6 Prandtl No.						
100	1.388331	30.575327	0.830673	22.64707	0.779934			
200	1.354983	38.467888	0.653625	33.98047	0.728049			
300	0 1.37667 45.929626 0.539934 47.43884 0.717399							
400	400 1.407398 53.462521 0.459245 62.98547 0.720053							
500	1.441664 60.805946 0.399644 79.74573 0.729673							
600	1.478299 67.710686 0.354492 96.22054 0.73976							
700	1.511776	74.211136	0.318248	119.118	0.750493			

Table 13: Results of \emptyset = 1.4 [for Reactants]

equivalence ratio = 1.4 for reactant								
The coeff. of nitrogen is $= 1.880952$								
The total mass of reactants is $= 71.466667$								
The mass	fraction of h	ydrogen is = ().039179					
The mass	fraction of or	xygen is $= 0.2$	23881					
The mass	fraction of ni	trogen is $= 0$.	736940					
Temp	Sp.Heat.	Sp.Heat. Cond Density Vis.*10-6 Prandtl No.						
-128.9	1.469599	0.016893	2.370008	5.239104	0.752591			
-17.8	1.526213	0.028278	1.340061	16.30015	0.728185			
93.4	1.542071	0.037268	0.931946	27.46353	0.717006			
204.4	204.4 1.559748 0.046077 0.717829 42.94832 0.7139							
315.6	315.6 1.583666 0.054568 0.580089 61.36297 0.71396							
426.7	1.610084	0.062257	0.481837	82.57221	0.715069			
537.8	1.636539 0.069215 0.421703 100.6049 0.71977							
538.9	1.662994 0.075465 0.358762 132.2814 0.731757							
760	1.68945 0.081013 0.331404 152.8705 0.742968							

equival	equivalence ratio 1.4 for product						
Enter cl	Enter choice= 1 for equivalence ratio = 1						
and 2 fo	or eq. ratio >	1 and 3 for eq.	. ratio < 1 3				
The coe	eff. of nitrog	en is = 1.88100	00				
The tota	al mass of pi	roducts is $= 71.4$	468002				
The ma	ss fraction o	f water is $= 0.2$	51861				
The ma	ss fraction o	f hydrogen is =	0.011194				
The ma	The mass fraction of nitrogen is $= 0.736945$						
Temp	Sp.Heat	Heat Cond.*10-3 Density Vis.*10-6 Prandtl No.					
100	1.461397	31.603226	6 0.826392 23.42214 0.7794				
200	1.428487	428487 39.71307 0.650258 35.11225 0.727763					
300	300 1.450256 47.133923 0.537154 48.99497 0.717085						
400	00 1.481034 54.867001 0.456875 65.14834 0.719724						
500	1.515142 62.572712 0.397556 82.08106 0.729275						
600	1.551697 69.589256 0.352665 99.25295 0.739329						
700	1.585189	76.201775	0.316608	122.9008	0.750049		

Table 14: Results of \emptyset = 1.4 [for Products]

 Table 15: Properties of Hydrogen [1, 5]

International Symbol		H2
Molecular weight		2.016
Specific gravity of gas at 32 F and 1 aim (air = 1)		0.06950
Specific volume at 70 F and 1 atm, cu ft/lb		192.0
Density of gas at 70 F and 1 atm, Ib/cu ft		0.005209
Density of gas at boiling point and 1 atm, Ib/cu ft		0.084
Density of liquid at boiling point and 1 arm, Ib/cu ft		4.428
Liquid/gas ratio		
(liquid at boiling point, gas at 70 F and 1 atm),vol/vol		1/850.1
Boiling point at 1 atm		- 423.0 F
Freezing point at 1 atm		- 434.6 F
Critical temperature		- 399.91 F
Critical pressure, psia		190.8
Triple point		-434.56F at 1.0414 psia
Latent heat of vaporization at boiling point, Btu/lb		192.7
Specific heat, <i>Cp</i> , at 70 F. Btu/(lb)(°F)		3.416
Specific heat, Cu. at 70 F. Btu/(lb)(°F)		2.430
Ratio of specific heats, Cp/Cu, at 70 F		1.41
Heat of combustion, Btu/cu ft		
	Gross	325
	Net	275
Solubility in water at 60 F. vol/1 vol of water		0.019
Weight per gallon, liquid, at boiling point, lb		0.5920

Results of Reactants at Different Equivalence Ratios $[\phi = 0.2 \text{ TO } 1.4]$



Figure 1: Specific Heat v/s Temperature for Reactants for $\phi = 0.2$ to 1.4



Figure 2: Thermal Conductivity v/s Temperature for Reactants for $\phi = 0.2$ to 1.4





Figure 3: Density v/s Temperature for Reactants for $\phi = 0.2$ to 1.4

Kinematic Viscosity for Reactant for $\varphi=0.2$ to 1.4



Figure 4: Kinematics Viscosity v/s Temperature for Reactants for $\phi = 0.2$ to 1.4

Prandi Number

0.76 0.75 0.74 0.73 0.72 0.72 0.72 0.72 0.72 0.72 0.72 0.72 0.72 0.75 0.72 0.75

Prandtl Number for Reactant for $\varphi=0.2$ to 1.4

◆phi=0.2 [■]phi=0.4 [▲]phi=0.6 [×]phi=0.8 [×]phi=1.0 ● phi=1.2 ⁺phi=1.4

Figure 5: Prandtl No. v/s Temperature for Reactants for $\phi = 0.2$ to 1.4

RESULTS OF THE PRODUCTS AT DIFFERENT EQUIVALENCE RATIOS [$\phi = 0.2$ TO 1.4]

Specific Heat for Product for φ =0.2 to 1.4



 $Specific \cdot Heat \cdot v/s \cdot Temperature \cdot for \cdot Products \cdot for \cdot \varphi = \cdot 0.2 \cdot To \cdot 1.4 \P$

Figure 6: Specific Heat v/s Temperature for Products for $\phi = 0.2$ To 1.4

Thermal conductivity for Product for φ=0.2 to 1.4



Figure 7: Thermal Conductivity v/s Temperature for Products for $\phi = 0.2$ to 1.4

Density for Product for $\varphi = 0.2$ to 1.4



Figure 8: Density v/s Temperature for Products for $\phi = 0.2$ to 1.4





Figure 9: Kinematics Viscosity v/s Temperature for Products for $\phi = 0.2$ to 1.4

Prandtl Number for Product for φ=0.2 to1.4



Figure 10: Prandtl No. v/s Temperature for Products for $\phi = 0.2$ to 1.4

MASS FRACTION OF REACTANT DIFFERENT EQUIVALENCE RATIOS

Table 16: Mass Fraction of Reactant at Different Equivalence Ratios

Φ	$\mathbf{H}_{2\mathbf{r}}$	O _{2r}	N_{2r}	Total Reactant[Kg/mole]
0.2	0.005792	0.2316	0.7625	345.33
0.4	0.01151	0.2303	0.7581	173.66

0.6	0.0171	0.229	0.7538	116.43
0.8	0.0227	0.2277	0.7459	87.8333
1	0.0283	0.2264	0.7452	70.6666
1.2	0.0337	0.2251	0.741	71.0666
1.4	0.03917	0.2238	0.7369	71.466



Figure 11: Variation of Mass Fraction of H2, O2 & N2 with Respect to Different Equivalence Ratio for Reactant

MASS FRACTION OF PRODUCT AT DIFFERENT EQUIVELENCE RATIOS

Ф	H_2O_p	O _{2p}	N_{2p}	$\mathbf{H}_{2\mathbf{p}}$	Total Product[Kg/mole]
0.2	0.05212	0.1853	0.7625	0	345.33
0.4	0.091	0.2429	0.6659	0	173.66
0.6	0.1481	0.0877	0.7641	0	116.43
0.8	0.196	0.0871	0.7168	0	87.8333
1	0.2547	0	0.7452	0	70.6666
1.2	0.2532	0	0.741	0.005628	71.0666
1.4	0.2518	0	0.7369	0.0111	71.466

Table 17: Mass Fraction of Product at Different Equivalence Ratios



Figure 12: Variation of Mass Fraction of H₂O, H2, O2 & N2 with Respect to Different Equivalence Ratio for Product