

COMPARITIVE STUDY OF SPECIES ANALYSIS OF SEMI-CRYOGENIC PROPELLANTS

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Abstract— Different computational software's were used for species analysis of various semi-cryogenic propellants. After analyzation the ideal and estimated values of various different parameters were calculated. Rocket Propulsion Analysis, a software developed by NASA was used for computing the ideal and estimated values as well as plotting of graphs with respect to different species. The adiabatic temperature of the species was also calculated by performing calculations on Microsoft Excel. In the end 1,1,1,2-tetrafluoroethane, a semi-cryogenic propellant was used in order to draw comparison with other species such as Hydrogen, Methane, RPA-1. Graphical representation of the main variables such as pressure, temperature, density, specific heat etc. with respect to the different nozzle positions was also done.

Keywords— Cryogenics, Cryogenic Engines, Cryogenic Propellants, Semi-Cryogenic Propellants, Species Analysis, RPA Analysis, Hydrogen (H_2), Methane (CH_4), RP1($C_{13}H_{28}$), 1,1,1,2-Tetra Floro Ethane (CH_2FCF_3).

INTRODUCTION

The branch of physics dealing with the production of very low temperature as well as their effect on matter is known as cryogenics. In Cryogenics the gas is cooled by compressing the gas, which in turn releases heat and later when allowed to expand produces ultra-low temperatures. Cooling can also be accomplished by magnetocaloric effect which is a magneto thermodynamic phenomenon in which exposing the material to a changing magnetic field causes a change in temperature. Cryogenic propellant is a type of liquid propellant that is kept at very low temperatures to remain liquid [1]. The commonest examples are liquid hydrogen(LH_2) and liquid oxygen(LOX). Special insulated containers and vents are used to store Cryogenic propellants in order to allow gas from the evaporating liquids to escape. Liquid fuel and oxidizer from the storage tanks are fed to an expansion chamber and then injected into the combustion chamber with proper feeding system, where they are further mixed and ignited by a flame or spark.

Low temperatures of cryogenic propellants make them difficult to store over long periods of time. For example, LH_2 has a very low density (0.59 pounds per gallon) and therefore, requires a storage volume greater than other fuels. The high efficiency of cryogenic propellants despite these drawbacks makes them the ideal choice, when reaction time and storability are not too critical.

United States of America in 1963 was the first country to develop the Cryogenic Rocket Engine (CRE) with the use of RL 10 engines employed on Atlas-V rocket [2]. Indian Space and Research Organization (ISRO) plans to develop a 2000 Kn Semi Cryogenic Engine (SCE) using LOX and ISROSENE (propellant-grade kerosene) for space applications. LOX and Kerosene are environmentally friendly and low-cost propellants. This Semi-Cryogenic engine will be used as the booster engine for the Common Liquid Core of the future heavy-lift Unified Launch Vehicles (ULV) and Reusable Launch Vehicles (RLV).

The liquid stages of PSLV and GSLV engines use toxic propellants that are harmful to the environment. The drift across the globe is to change over to eco-friendly propellants [3]. The green propellant candidates are plentiful and include combinations like LOX - LH_2 and LOX - pure hydrocarbons. 1,1,1,2-Tetrafluoroethane also known as norflurane (INN), is a halo alkane refrigerant with insignificant ozone depletion potential and a lower global warming potential [4][5]. 1,1,1,2-Tetrafluoroethane is a non-flammable gas whose other uses include plastic foam blowing, cleaning solvent, etc. It is also used as a solvent in organic chemistry, both in liquid and supercritical fluid. It is also used for other types of particle detectors. [6][7].

LITERATURE SURVEY

CRYOGENIC ROCKET ENGINE

A rocket engine that uses cryogenic fuel or oxidizer is known as a cryogenic rocket engine. Its fuel or oxidizer (or both) are gases that are liquefied and stored at very low temperatures. These engines require high mass flow rate of both oxidizer and fuel to generate sufficient thrust. Oxygen and low molecular weight hydrocarbons are used as oxidizer and fuel pair. They are in gaseous state at room temperature and pressure. Theoretically, if we store propellants as pressurized gases, the size and mass of the tanks would severely decrease rocket efficiency, therefore in order to get the required mass flow rate the propellants must be cooled down to cryogenic temperatures (below -150°C , -238°F)[8]. This converts them from gaseous state to liquid state. All cryogenic rocket engines by definition are, either liquid-propellant rocket engines or hybrid rocket engines. The most widely used combination amongst the numerous cryogenic fuel-oxidizer combinations is that of liquid hydrogen (LH_2) as fuel and liquid oxygen (LOX) as oxidizer. These components when burned have one of the maximum entropy releases by combustion. They produce a specific impulse up to 450 s with an effective exhaust velocity of 4.4 km/s [9].



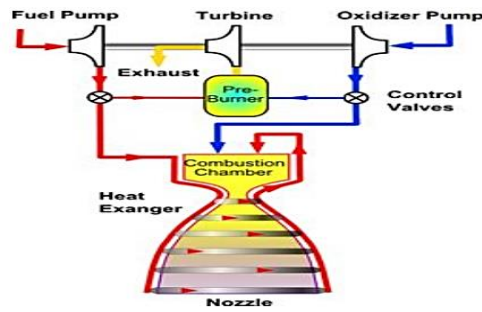
(Fig.1 Cryogenic engine /Source: Cryogenic Technology Development for Exploration Missions by David J. Chato)

COMPONENTS

Cryogenic rocket engine comprises of a combustion chamber, fuel cryopumps, oxidizer cryopumps, gas turbine, cryo valves, regulators, pyrotechnic igniter, fuel injector, fuel tanks, and rocket engine nozzle. Cryogenic rocket engines work in either an expander cycle, a gas generator cycle, a staged combustion cycle, or the simplest pressure-fed cycle in order to feed the propellants to the combustion chamber. Looking at this aspect, engines can be differentiated into a main flow or a bypass flow configuration [10].

WORKING

Cryogenic Engines are rocket motors that are designed for liquid fuels held at cryogenic temperatures. Hydrogen and Oxygen are used typically which need to be held below 20°K (-423°F) and 90°K (297°F) in order to remain liquid. The engine components are also cooled so that the fuel doesn't boil and change to gaseous form in the feeding system. Thrust is generated due to the rapid expansion from liquid to gaseous state, with the gas emerging from the motor at very high speed. Cryogenic engines are the highest performing rocket motors. However, one disadvantage of cryogenic engines is that the fuel tanks tend to be bulky since they require heavy insulation to store the propellant. This disadvantage is however compensated by their high fuel efficiency. Ariane 5 uses oxygen and hydrogen, both stored as a cryogenic liquid, to produce its power. Liquid nitrogen, stored at -320 degrees Fahrenheit, is vaporized with the help of heat exchanger. Nitrogen gas formed in the heat exchanger then expands to about 700 times the volume of its liquid form. The force of the nitrogen gas is converted into mechanical power when the highly pressurized gas is fed to the expander.



(Fig.2 Working principle of cryogenic engine /

Source; Richard Cohn, *Developments in Liquid Rocket Engine Technology*, Air Force Research Laboratory, 2012.)

CRYOGENIC PROPELLANTS

The fuel and the oxidizer are in the form of very cold, liquefied gases in a cryogenic propellant. Since they stay in liquid form even though they are at a temperature lower than their freezing point these liquefied gases are referred to as super cooled. Thus cryogenic fuels are super cooled gases used as liquid fuels. These propellants however are gases at normal atmospheric conditions. Because of their very low densities storing these propellants aboard a rocket is a very difficult task. Hence in order to store the propellants extremely huge tanks are required. Although their density can be increased by cooling and compressing them into liquids hence, making it possible to store them in large quantities in smaller tanks. The propellant combination of liquid oxygen and liquid hydrogen is normally used, Liquid oxygen being the oxidizer and liquid hydrogen being the fuel. [11].

CRYOGEN	TRIPLE POINT [k]	NORMAL B.P. [k]	CRITICAL POINT [k]
METHANE (CH₄)	90.7	111.6	190.5
OXYGEN (O₂)	54.4	90.2	154.6
ARGON	83.3	87.3	150.9
NITROGEN	63.1	77.3	126.2
NEON	24.6	27.1	44.4
HYDROGEN (H₂)	13.8	20.4	33.2
HELIUM	2.2	4.2	5.2

(TABLE 1; Characteristic Temperature of Cryogenic fluids;

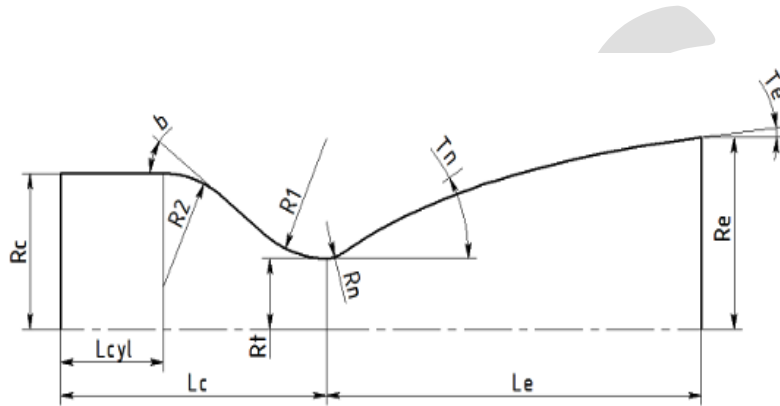
Source; *International Journal of Aerospace and Mechanical Engineering Volume 2 – No.5, August 2015, Cryogenic Technology & Rocket Engines*)

The trend worldwide is to change over to eco-friendly propellants. Already known combinations like LOX - LH2 and LOX - pure hydrocarbons are amongst the numerous green propellant candidates. Solid propellant boosters could be also replaced by green liquid propellants but green solid candidates exist also. A first review of candidate chemical products revealed that no perfect green exist. The maximum allowable concentration in air for workers is sometimes very low for some green candidates. Other can form very easily explosive mixtures with air. Some risks should be accepted when greens are selected and they could be mitigated by appropriate measures.

ROCKET PROPULSION ANALYSIS (RPA)

RPA stands for Rocket Propulsion Analysis. It is an easy-to-use multi-platform tool used for the performance prediction of rocket engines. Along with convenient grouping of the input parameters and analysis results it also features an intuitive graphical user interface. Based on NASA's Glenn thermodynamic database RPA utilizes an expandable chemical species library. This library includes data for numerous fuels and oxidizers, such as liquid hydrogen and oxygen, kerosene, hydrogen peroxide and many others. The users can also easily define new propellant components, or import components from PROPEP or CEA2 species databases with embedded species editor.

The program obtains chemical equilibrium composition of combustion products by providing a few engine parameters such as combustion chamber pressure, used propellant components, and nozzle parameters, as well as determines its thermodynamic properties. It also predicts the theoretical rocket performance. These calculations are used in the designing process of combustion chambers, gas generators and preburners. Based on robust, proven and industry-accepted Gibbs free energy minimization approach the calculation method is used to obtain the combustion composition. Further analysis of nozzle flows with shifting and frozen chemical equilibrium, and calculation of engine performance for a finite and infinite-area combustion chambers is also done. RPA is written in C++ programming language using following libraries: Qt, Qwt, libconfig++ [12][13]. * Ambient condition for optimum expansion: $H=0.00$ km, $p=1.000$ atm.



R_c ; Chamber radius

L_{cyl} ; Length of cylinder

R_2 ; Contraction of throat radius

B ; Contraction angle

R_t ; Throat radius

L_c ; Distance from start of nozzle to throat

R_1 ; Radius of throat profile

R_n ; Projected radius

T_n ; Divergent angle

L_e ; Distance from throat to exit nozzle

R_e ; Exit radius

T_e ; Exit angle

(Fig 3. Contour of exhaust nozzle; Source: RPA Analysis)

HYDROGEN (H₂)

Component	Temperature (K)	Mass fraction	Mole fraction
H ₂ (L)	20.27	0.18	0.77
O ₂ (L)	90.17	0.82	0.23
Total		1.00	1.00

Exploded propellant formula:	O _{0.455} H _{1.545}
O/F =	4.672
O/F⁰ =	7.937 (stoichiometric)
α_{ox} =	0.589 (oxidizer excess coefficient)

(Table 3: Propellant Specification; Source: RPA Analysis)

Species	Injector	Injector	Nozzle inlet	Nozzle inlet	Nozzle throat	Nozzle throat	Nozzle exit	Nozzle exit
	mass fractions	mole fractions	mass fractions	mole fractions	mass fractions	mole fractions	mass fractions	mole fractions
<i>H</i>	0.001413	0.015825	0.001413	0.015825	0.000919	0.010344	1E-07	1.4E-06
<i>H₂</i>	0.072028	0.403252	0.072028	0.403252	0.072095	0.40569	0.072519	0.411333
<i>H₂O</i>	0.911701	0.571154	0.911701	0.571154	0.918903	0.578609	0.927481	0.588666
<i>H₂O₂</i>	5.4E-06	1.8E-06	5.4E-06	1.8E-06	1.8E-06	6E-07		
<i>HO₂</i>	5.5E-06	1.9E-06	5.5E-06	1.9E-06	1.5E-06	5E-07		
<i>O</i>	0.00029	0.000205	0.00029	0.000205	0.000106	7.53E-05		
<i>O₂</i>	0.000321	0.000113	0.000321	0.000113	0.00012	4.25E-05		
<i>OH</i>	0.014237	0.009448	0.014237	0.009448	0.007855	0.005239		

(Table 4. Fractions of the combustion products; Source: RPA Analysis)

Parameter	Injector	Nozzle inlet	Nozzle throat	Nozzle exit	Unit
Pressure	15.0000	15.0000	8.5217	0.1013	MPa
Temperature	3230.2733	3230.2733	2982.6784	1345.8039	K
Enthalpy	-1122.2620	-1122.2620	-2412.6981	-9208.9043	kJ/kg
Entropy	19.4372	19.4372	19.4372	19.4372	kJ/(kg·K)
Internal energy	-3502.0145	-3502.0145	-4598.8717	-10187.5188	kJ/kg
Specific heat (p=const)	6.0388	6.0388	5.4520	3.4860	kJ/(kg·K)
Specific heat (V=const)	5.1144	5.1144	4.5998	2.7588	kJ/(kg·K)
Gamma	1.1807	1.1807	1.1853	1.2636	
Isentropic exponent	1.1730	1.1730	1.1805	1.2636	
Gas constant	0.7367	0.7367	0.7330	0.7272	kJ/(kg·K)
Molecular weight (M)	11.2861	11.2861	11.3437	11.4342	
Molecular weight (MW)	0.01129	0.01129	0.01134	0.01143	

Density	6.3032	6.3032	3.8980	0.1035	kg/m ³
Sonic velocity	1670.7359	1670.7359	1606.5095	1112.0076	m/s
Velocity	0.0000	0.0000	1606.5095	4021.6022	m/s
Mach number	0.0000	0.0000	1.0000	3.6165	
Area ratio	infinity	infinity	1.0000	15.0390	
Mass flux	0.0000	0.0000	6262.1399	416.3936	kg/(m ² ·s)
Mass flux (relative)	0.000e-04	0.000e-04			kg/(N·s)
Viscosity	9.575e-05	9.575e-05	9.033e-05	4.855e-05	kg/(m·s)
Conductivity, frozen	0.6134	0.6134	0.5689	0.2625	W/(m·K)
Specific heat (p=const), frozen	4.316	4.316	4.256	3.486	kJ/(kg·K)
Prandtl number, frozen	0.6737	0.6737	0.6758	0.6446	
Conductivity, effective	1.087	1.087	0.8943	0.2626	W/(m·K)
Specific heat (p=const), effective	6.039	6.039	5.452	3.486	kJ/(kg·K)
Prandtl number, effective	0.5321	0.5321	0.5506	0.6445	

(Table 5. Thermodynamic properties; Source: RPA Analysis)

Parameter	Sea level	Optimum expansion	Vacuum	Unit
Characteristic velocity		2395.35		m/s
Effective exhaust velocity	4021.60	4021.60	4264.94	m/s
Specific impulse (by mass)	4021.60	4021.60	4264.94	N·s/kg
Specific impulse (by weight)	410.09	410.09	434.90	s
Thrust coefficient	1.6789	1.6789	1.7805	

(Table 6. Theoretical (ideal) performance; Source: RPA Analysis)

Parameter	Sea level	Optimum expansion	Vacuum	Unit
Characteristic velocity		2390.91		m/s
Effective exhaust velocity	3913.47	3913.47	4156.81	m/s
Specific impulse (by mass)	3913.47	3913.47	4156.81	N·s/kg
Specific impulse (by weight)	399.06	399.06	423.88	s
Thrust coefficient	1.6368	1.6368	1.7386	

(Table 7. Estimated delivered performance; Source: RPA Analysis)

METHANE (CH₄)

Component	Temperature (K)	Mass fraction	Mole fraction
CH₄(L)	111.64	0.23	0.37
O₂(L)	90.17	0.77	0.63
Total		1	1
Exploded propellant formula:	O _{1.252} C _{0.374} H _{1.495}		
O/F =	3.341		

$O/F^0 =$	3.989 (stoichiometric)		
$\alpha_{ox} =$	0.837 (oxidizer excess coefficient)		

(Table 8: Propellant Specification; Source: RPA Analysis)

Parameter	Injector	Nozzle inlet	Nozzle throat	Nozzle exit	Unit
Pressure	10	10	5.7838	0.1013	MPa
Temperature	3590.9374	3590.9374	3411.3432	2191.902	K
Enthalpy	-1593.6405	-1593.6405	-2326.6326	-6502.1	kJ/kg
Entropy	12.0987	12.0987	12.0987	12.0987	kJ/(kg·K)
Internal energy	-2975.6995	-2975.6995	-3623.2121	-7288.6	kJ/kg
Specific heat (p=const)	6.6033	6.6033	6.3784	2.4822	kJ/(kg·K)
Specific heat (V=const)	5.6286	5.6286	5.4759	2.1053	kJ/(kg·K)
Gamma	1.1732	1.1732	1.1648	1.179	
Isentropic exponent	1.1335	1.1335	1.1307	1.178	
Gas constant	0.3849	0.3849	0.3801	0.3588	kJ/(kg·K)
Molecular weight (M)	21.6031	21.6031	21.8756	23.1716	
Molecular weight (MW)	0.0216	0.0216	0.02188	0.02317	
Density	7.2356	7.2356	4.4608	0.1288	kg/m ³
Sonic velocity	1251.6157	1251.6157	1210.7803	962.5474	m/s
Velocity	0	0	1210.7803	3133.196	m/s
Mach number	0	0	1	3.2551	
Area ratio	infinity	infinity	1	13.3805	
Mass flux	0	0	5401.0443	403.6499	kg/(m ² ·s)
Mass flux (relative)	0.00E+00	0.00E+00			kg/(N·s)
Viscosity	0.000114	0.000114	0.0001103	8.16E-05	kg/(m·s)
Conductivity, frozen	0.396	0.396	0.3782	0.2502	W/(m·K)
Specific heat (p=const), frozen	2.348	2.348	2.336	2.191	kJ/(kg·K)
Prandtl number, frozen	0.6759	0.6759	0.681	0.7147	
Conductivity, effective	1.387	1.387	1.276	0.3145	W/(m·K)
Specific heat (p=const), effective	6.603	6.603	6.378	2.482	kJ/(kg·K)
Prandtl number, effective	0.5428	0.5428	0.551	0.644	

(Table 9. Thermodynamic properties; Source: RPA Analysis)

Species	Injector	Injector	Nozzle inlet	Nozzle inlet	Nozzle throat	Nozzle throat	Nozzle exit	Nozzle exit
	mass fractions	mole fractions	mass fractions	mole fractions	mass fractions	mole fractions	mass fractions	mole fractions
CO	0.2381517	0.1836771	0.2381517	0.183677	0.227494	0.177671	0.1666726	0.137882
CO2	0.2577548	0.1265249	0.2577548	0.126525	0.274536	0.136463	0.3701455	0.194887
COOH	0.0000392	0.0000188	0.0000392	1.88E-05	2.27E-05	0.000011		
H	0.0009841	0.0210931	0.0009841	0.021093	0.000833	0.018087	0.0000654	0.001503
H2	0.0079433	0.085124	0.0079433	0.085124	0.007528	0.081686	0.0068581	0.078831

H2O	0.4112356	0.4931347	0.4112356	0.493135	0.420785	0.510953	0.4548955	0.585096
H2O2	0.0000391	0.0000248	0.0000391	2.48E-05	2.27E-05	1.46E-05		
HCHO	0.0000009	0.0000007	0.0000009	7E-07	5E-07	4E-07		
HCO	0.0000238	0.0000177	0.0000238	1.77E-05	1.29E-05	9.8E-06		
HCOOH	0.0000075	0.0000035	0.0000075	3.5E-06	4.2E-06	0.000002		
HO2	0.0001861	0.0001218	0.0001861	0.000122	0.000111	7.39E-05		
O	0.00624	0.0084255	0.00624	0.008426	0.004687	0.006409	0.0000141	2.04E-05
O2	0.0276826	0.0186891	0.0276826	0.018689	0.022651	0.015485	0.000088	6.37E-05
O3	0.0000002	0.0000001	0.0000002	1E-07				
OH	0.0497109	0.0631438	0.0497109	0.063144	0.04131	0.053135	0.0012605	0.001717

(Table 10. Fractions of the combustion products; Source: RPA Analysis)

Parameter	Sea level	Optimum expansion	Vacuum	Unit
Characteristic velocity		1851.49		m/s
Effective exhaust velocity	3133.2	3133.2	3384.22	m/s
Specific impulse (by mass)	3133.2	3133.2	3384.22	N·s/kg
Specific impulse (by weight)	319.5	319.5	345.09	s
Thrust coefficient	1.6923	1.6923	1.8278	

(Table 11. Theoretical (ideal) performance; Source: RPA Analysis)

Parameter	Sea level	Optimum expansion	Vacuum	Unit
Characteristic velocity		1826.69		m/s
Effective exhaust velocity	3008.78	3008.78	3259.8	m/s
Specific impulse (by mass)	3008.78	3008.78	3259.8	N·s/kg
Specific impulse (by weight)	306.81	306.81	332.41	s
Thrust coefficient	1.6471	1.6471	1.7845	

(Table 12. Estimated delivered performance; Source: RPA Analysis)

RP1(C₁₃H₂₈)

Component	Temperature (K)	Mass fraction	Mole fraction
RP-1	298.15	0.27	0.46
O ₂ (L)	90.17	0.73	0.54
Total		1.00	1.00

Exploded propellant formula:	$O_{1.083} C_{0.458} H_{0.894}$
O/F =	2.704
α_{ox} =	0.794 (oxidizer excess coefficient)
O/F⁰ =	3.406 (stoichiometric)

(Table 13: Propellant Specification; Source: RPA Analysis)

Parameter	Injector	Nozzle inlet	Nozzle throat	Nozzle exit	Unit
Pressure	10.0000	10.0000	5.7793	0.1013	MPa
Temperature	3740.7309	3740.7309	3553.8958	2354.4877	K
Enthalpy	-773.5330	-773.5330	-1462.4738	-5389.633	kJ/kg
Entropy	11.0335	11.0335	11.0335	11.0335	kJ/(kg·K)
Internal energy	-2071.588	-2071.588	-2678.6198	-6139.435	kJ/kg
Specific heat (p=const)	6.3447	6.3447	6.2320	2.4608	kJ/(kg·K)
Specific heat (V=const)	5.3499	5.3499	5.2979	2.1040	kJ/(kg·K)
Gamma	1.1860	1.1860	1.1763	1.1695	
Isentropic exponent	1.1370	1.1370	1.1330	1.1670	
Gas constant	0.3470	0.3470	0.3422	0.3185	kJ/(kg·K)
Molecular weight (M)	23.9606	23.9606	24.2971	26.1087	
Molecular weight (MW)	0.02396	0.02396	0.0243	0.02611	
Density	7.7038	7.7038	4.7521	0.1351	kg/m ³
Sonic velocity	1214.8433	1214.8433	1173.8361	935.4050	m/s
Velocity	0.0000	0.0000	1173.8361	3038.4536	m/s
Mach number	0.0000	0.0000	1.0000	3.2483	
Area ratio	infinity	infinity	1.0000	13.5853	
Mass flux	0.0000	0.0000	5578.1922	410.6035	kg/(m ² ·s)
Mass flux (relative)	0.000e-04	0.000e-04			kg/(N·s)
Viscosity	0.0001149	0.0001149	0.0001111	8.418e-05	kg/(m·s)
Conductivity, frozen	0.355	0.355	0.3396	0.2354	W/(m·K)
Specific heat (p=const), frozen	2.019	2.019	2.011	1.924	kJ/(kg·K)
Prandtl number, frozen	0.6537	0.6537	0.658	0.688	

Conductivity, effective	1.419	1.419	1.333	0.3623	W/(m·K)
Specific heat (p=const), effective	6.345	6.345	6.232	2.461	kJ/(kg·K)
Prandtl number, effective	0.5138	0.5138	0.5193	0.5718	

(Table 14. Thermodynamic properties; Source: RPA Analysis)

(Table

Species	Injector	Injector	Nozzle inlet	Nozzle inlet	Nozzle throat	Nozzle throat	Nozzle exit	Nozzle exit
	mass fractions	mole fractions	mass fractions	mole fractions	mass fractions	mole fractions	mass fractions	mole fractions
CO	0.3484917	0.298109	0.3484917	0.2981093	0.3354517	0.290984	0.260107	0.242449
CO2	0.3023635	0.164619	0.3023635	0.1646193	0.3229032	0.178271	0.441354	0.261833
COOH	0.0000529	2.82E-05	0.0000529	0.0000282	0.0000313	1.69E-05	3E-07	2E-07
H	0.0010981	0.026103	0.0010981	0.0261033	0.0009493	0.022883	0.000127	0.003297
H2	0.0059015	0.070145	0.0059015	0.0701451	0.0056439	0.068025	0.005212	0.0675
H2O	0.2507053	0.333442	0.2507053	0.333442	0.2582547	0.348306	0.290187	0.420554
H2O2	0.000032	2.25E-05	0.000032	0.0000225	0.0000191	1.37E-05		
HCHO	0.0000011	9E-07	0.0000011	0.0000009	0.0000006	5E-07		
HCO	0.0000389	3.21E-05	0.0000389	0.0000321	0.0000216	1.81E-05	2E-07	1E-07
HCOOH	0.0000075	3.9E-06	0.0000075	0.0000039	0.0000043	2.3E-06		
HO2	0.0002046	0.000149	0.0002046	0.0001485	0.000127	9.35E-05	2E-07	2E-07
O	0.0091408	0.013689	0.0091408	0.0136892	0.0071031	0.010787	7.16E-05	0.000117
O2	0.0330513	0.024749	0.0330513	0.0247487	0.0279008	0.021185	0.000371	0.000302
O3	0.0000004	2E-07	0.0000004	0.0000002				
OH	0.0489102	0.068907	0.0489102	0.0689066	0.0415892	0.059415	0.002571	0.003947

Fractions of the combustion products; Source: RPA Analysis]

15.

Parameter	Sea level	Optimum expansion	Vacuum	Unit
<i>Characteristic velocity</i>		1792.70		m/s
<i>Effective exhaust velocity</i>	3038.45	3038.45	3285.22	m/s
<i>Specific impulse (by mass)</i>	3038.45	3038.45	3285.22	N·s/kg
<i>Specific impulse (by weight)</i>	309.84	309.84	335.00	s
<i>Thrust coefficient</i>	1.6949	1.6949	1.8326	

(Table 16. Theoretical (ideal) performance; Source: RPA Analysis)

Parameter	Sea level	Optimum expansion	Vacuum	Unit
<i>Characteristic velocity</i>		1770.67		m/s
<i>Effective exhaust velocity</i>	2921.29	2921.29	3168.06	m/s
<i>Specific impulse (by mass)</i>	2921.29	2921.29	3168.06	N·s/kg
<i>Specific impulse (by weight)</i>	297.89	297.89	323.05	s
<i>Thrust coefficient</i>	1.6498	1.6498	1.7892	

(Table 17. Estimated delivered performance; Source: RPA Analysis)

1,1,1,2-TETRA FLORO ETHANE (CH₂FCF₃)

Parameter	Sea level	Optimum expansion	Vacuum	Unit
<i>Characteristic velocity</i>		1856.2		m/s
<i>Effective exhaust velocity</i>	3112.32	3112.32	3363.33	m/s
<i>Specific impulse (by mass)</i>	3112.32	3112.32	3363.33	N·s/kg
<i>Specific impulse (by weight)</i>	317.37	317.37	342.96	s
<i>Thrust coefficient</i>	1.6767	1.6767	1.8119	
<i>Characteristic velocity</i>		1830.91		m/s
<i>Effective exhaust velocity</i>	2987.92	2987.92	3238.93	m/s
<i>Specific impulse (by mass)</i>	2987.92	2987.92	3238.93	N·s/kg
<i>Specific impulse (by weight)</i>	304.68	304.68	330.28	s
<i>Thrust coefficient</i>	1.6319	1.6319	1.769	

(Table 18. Theoretical (ideal) & Estimated delivered performance; Source: RPA Analysis)

Parameter	Injector	Nozzle inlet	Nozzle throat	Nozzle exit	Unit
<i>Pressure</i>	10	10	5.6395	0.1013	MPa
<i>Temperature</i>	4196.836	4196.836	3851.7631	2590.4963	K

Enthalpy	258.8972	258.8972	-535.4484	-4584.36	kJ/kg
Entropy	9.862	9.862	9.862	9.862	kJ/(kg·K)
Internal energy	-1198.423	-1198.423	-1854.882	-5365.586	kJ/kg
Specific heat (p=const)	2.9785	2.9785	3.2869	6.9664	kJ/(kg·K)
Specific heat (V=const)	2.3921	2.3921	2.6521	5.899	kJ/(kg·K)
Gamma	1.2451	1.2451	1.2394	1.1809	
Isentropic exponent	1.2135	1.2135	1.2041	1.1273	
Gas constant	0.3472	0.3472	0.3426	0.3016	kJ/(kg·K)
Molecular weight (M)	23.9443	23.9443	24.2721	27.5703	
Molecular weight (MW)	0.02394	0.02394	0.02427	0.02757	
Density	6.8619	6.8619	4.2742	0.1297	kg/m ³
Sonic velocity	1329.807	1329.807	1260.4322	938.4393	m/s
Velocity	0	0	1260.4322	3112.3166	m/s
Mach number	0	0	1	3.3165	
Area ratio	infinity	infinity	1	13.346	
Mass flux	0	0	5387.3535	403.6677	kg/(m ² ·s)
Mass flux (relative)	0.00E+00	0.00E+00			kg/(N·s)
Viscosity	0.000129	0.000129	0.0001217	9.16E-05	kg/(m·s)
Conductivity, frozen	0.2649	0.2649	0.2482	0.1773	W/(m·K)
Specific heat (p=const), frozen	1.454	1.454	1.444	1.414	kJ/(kg·K)
Prandtl number, frozen	0.7065	0.7065	0.7086	0.7307	
Conductivity, effective	0.5773	0.5773	0.5069	0.7119	W/(m·K)
Specific heat (p=const), effective	2.979	2.979	3.287	6.966	kJ/(kg·K)
Prandtl number, effective	0.6642	0.6642	0.7895	0.8967	

(Table 19. Thermodynamic properties: Source; RPA Analysis)

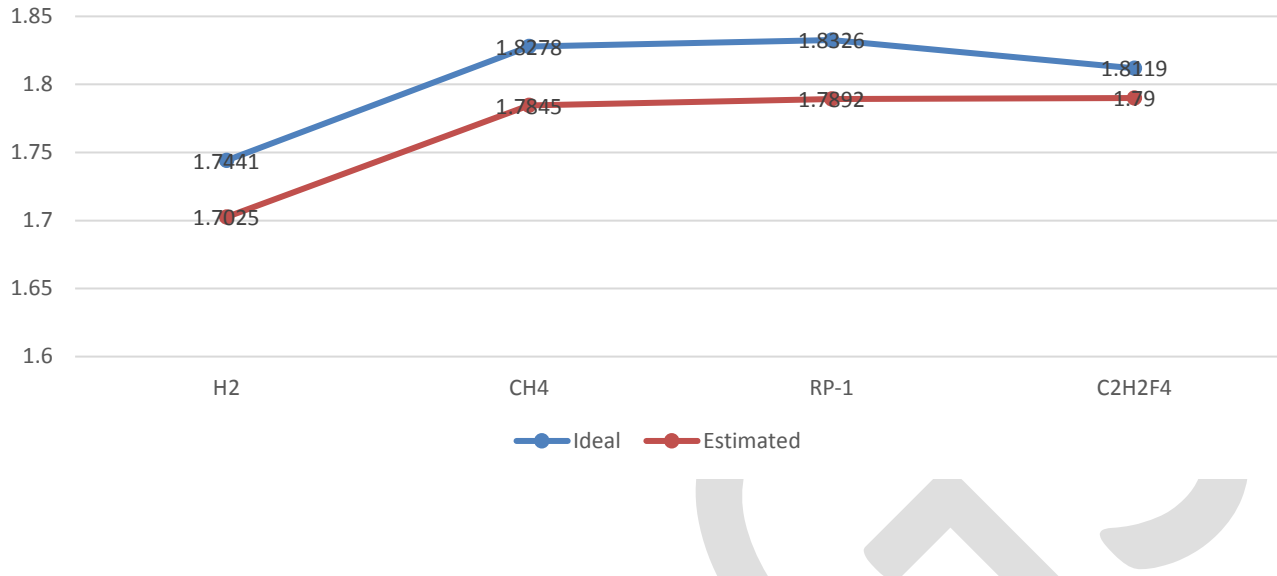
Species	Injector	Injector	Nozzle inlet	Nozzle inlet	Nozzle throat	Nozzle throat	Nozzle exit	Nozzle exit
	mass fractions	mole fractions	mass fractions	mole fractions	mass fractions	mole fractions	mass fractions	mole fractions
C	0.000054	0.000108	0.000054	0.0001076	1.29E-05	2.61E-05		

C2	1.29E-05	1.29E-05	0.0000129	0.0000129	0.000002	2.1E-06		
C2F	0.000314	0.000175	0.0003135	0.0001745	0.000114	6.41E-05		
C2F2	0.008911	0.003441	0.0089114	0.0034405	0.00747	0.002923	0.000138	6.14E-05
C2F3	1.71E-05	5.1E-06	0.0000171	0.0000051	1.19E-05	3.6E-06		
C2F4	7.3E-06	1.8E-06	0.0000073	0.0000018	9.9E-06	2.4E-06	5E-07	1E-07
C2F6							1.1E-06	2E-07
C2H	3.5E-06	3.4E-06	0.0000035	0.0000034	4E-07	4E-07		
C2H2,acetylene	3E-07	2E-07	0.0000003	0.0000002				
C2HF	0.00011	5.99E-05	0.0001101	0.0000599	3.58E-05	1.97E-05		
C2HF3	4E-07	1E-07	0.0000004	0.0000001				
C2O	2.37E-05	1.42E-05	0.0000237	0.0000142	0.000007	4.2E-06		
C3	9.9E-06	6.6E-06	0.0000099	0.0000066	1.4E-06	9E-07		
CF	0.020129	0.015543	0.0201294	0.0155433	0.011309	0.008852	0.000107	9.54E-05
CF+	4.4E-06	3.4E-06	0.0000044	0.0000034	1.4E-06	1.1E-06		
CF2	0.085608	0.04099	0.085608	0.0409903	0.097496	0.047321	0.024069	0.01327
CF3	0.00548	0.001902	0.0054799	0.0019015	0.008319	0.002926	0.004709	0.001881
CF3+	1.6E-06	6E-07	0.0000016	0.0000006	1.4E-06	5E-07		
CF4	0.002841	0.000773	0.0028408	0.0007729	0.009209	0.00254	0.19659	0.061588
CH	6E-07	1.1E-06	0.0000006	0.0000011	1E-07	1E-07		
CH2F	3E-07	2E-07	0.0000003	0.0000002				
CHF	7.63E-05	0.000057	0.0000763	0.000057	2.39E-05	1.82E-05		
CHF2	6.93E-05	3.25E-05	0.0000693	0.0000325	3.67E-05	1.75E-05		
CHF3	4.91E-05	1.68E-05	0.0000491	0.0000168	5.22E-05	1.81E-05	5.8E-06	2.3E-06
CO	0.356872	0.30507	0.3568719	0.3050699	0.356457	0.308886	0.353059	0.347515
CO2	6.62E-05	0.000036	0.0000662	0.000036	6.28E-05	3.46E-05	6.83E-05	4.28E-05
COF2	0.001972	0.000715	0.0019722	0.0007154	0.003333	0.001226	0.012443	0.005197
COHF	4.3E-06	2.1E-06	0.0000043	0.0000021	2.3E-06	1.2E-06		
F	0.20602	0.259654	0.2060201	0.2596535	0.193853	0.247664	0.096853	0.140552
F-	3.2E-06	0.000004	0.0000032	0.000004	1.3E-06	1.6E-06		
F2	0.000225	0.000142	0.0002253	0.000142	0.00018	0.000115	1.26E-05	9.1E-06
FCO	0.001078	0.000549	0.0010776	0.0005489	0.00086	0.000444	8.98E-05	5.27E-05
FO	3E-07	2E-07	0.0000003	0.0000002				
H	8.32E-05	0.001976	0.0000832	0.001976	3.34E-05	0.000804	4E-07	1.04E-05
H2	6.7E-06	7.97E-05	0.0000067	0.0000797	0.000002	2.45E-05		
H2F2	0.003893	0.00233	0.0038932	0.0023298	0.002273	0.001379	5.16E-05	3.56E-05
HCO	2.3E-06	1.9E-06	0.0000023	0.0000019	6E-07	5E-07		
HF	0.306036	0.366274	0.3060358	0.3662741	0.308823	0.374669	0.311801	0.429685
O	1.23E-05	1.84E-05	0.0000123	0.0000184	5.3E-06	0.000008	1E-07	2E-07
OH	0.000001	1.4E-06	0.000001	0.0000014	3E-07	5E-07		

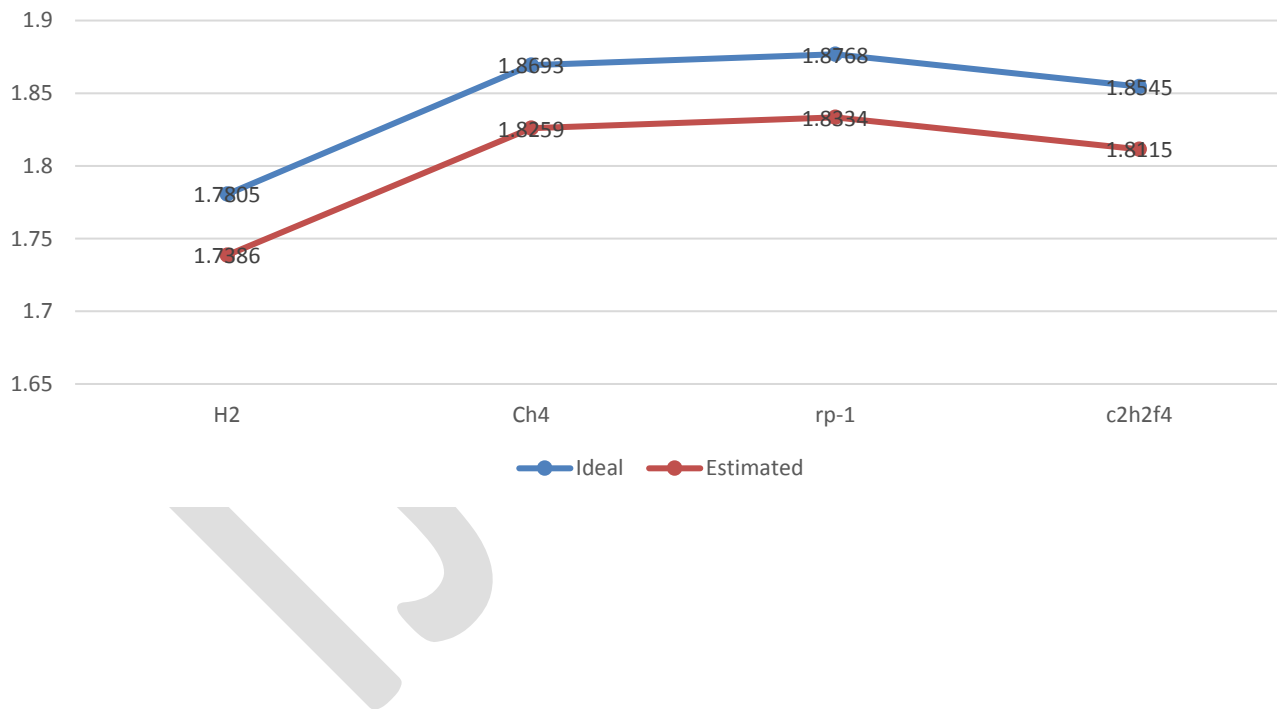
(Table 20. Fractions of the combustion products; Source; RPA Analysis)

RESULT

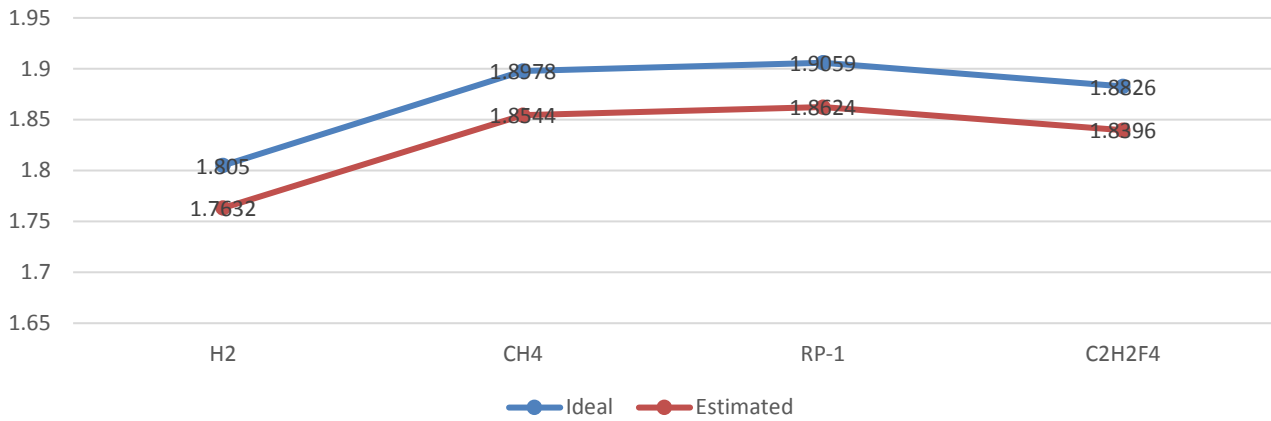
Thrust Coefficient in Vacuum at 10 Mpa



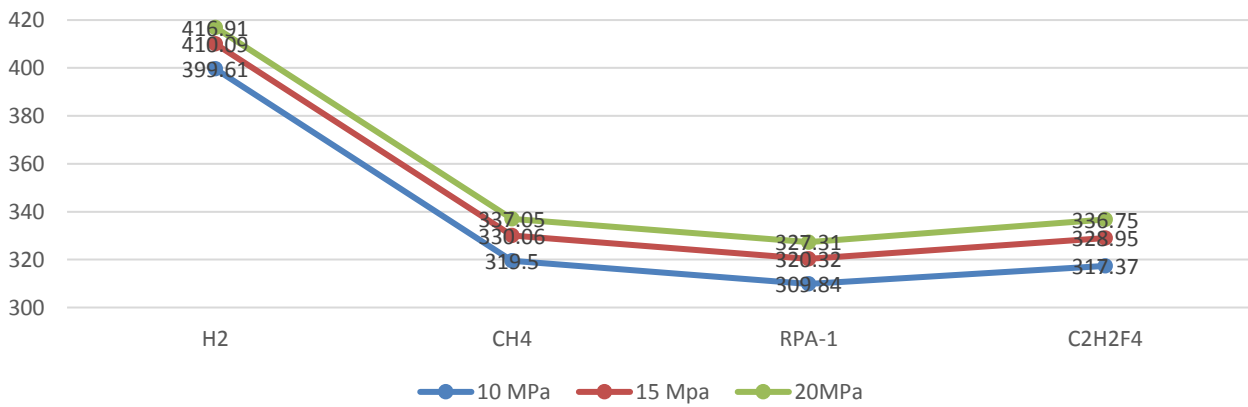
Thrust Coefficient in Vacuum at 15 Mpa



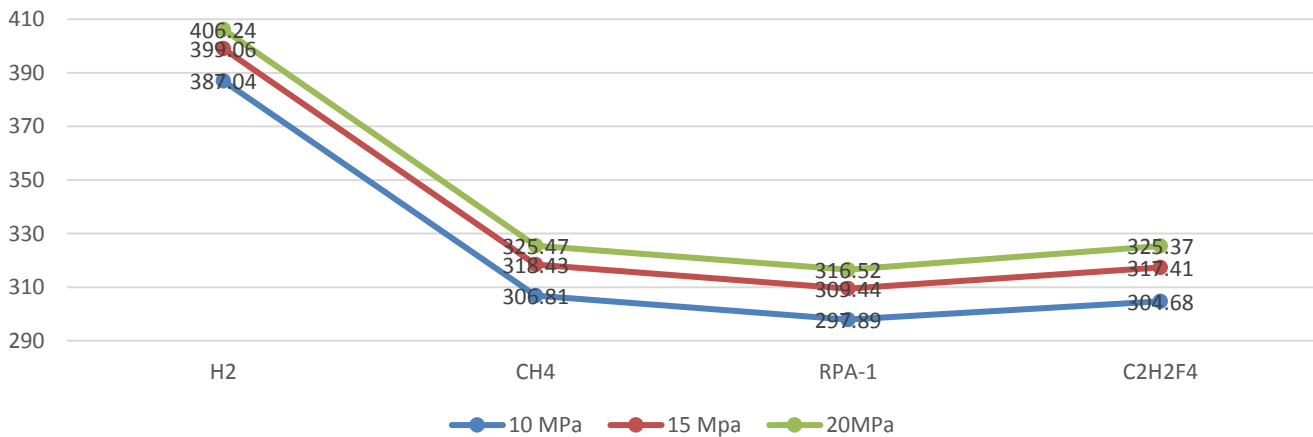
Thrust Coefficient in Vacuum at 20 Mpa



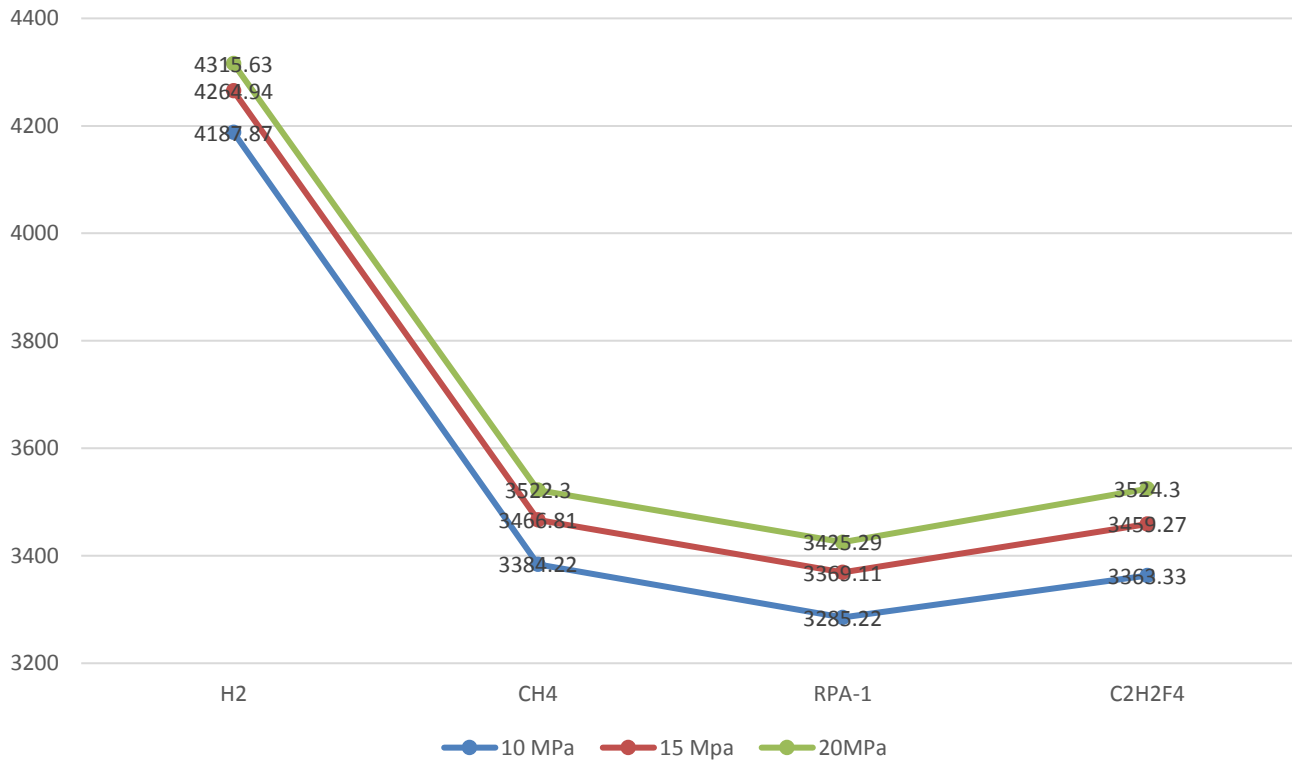
I_{sp} of fuels at different Chamber Pressure (Ideal)



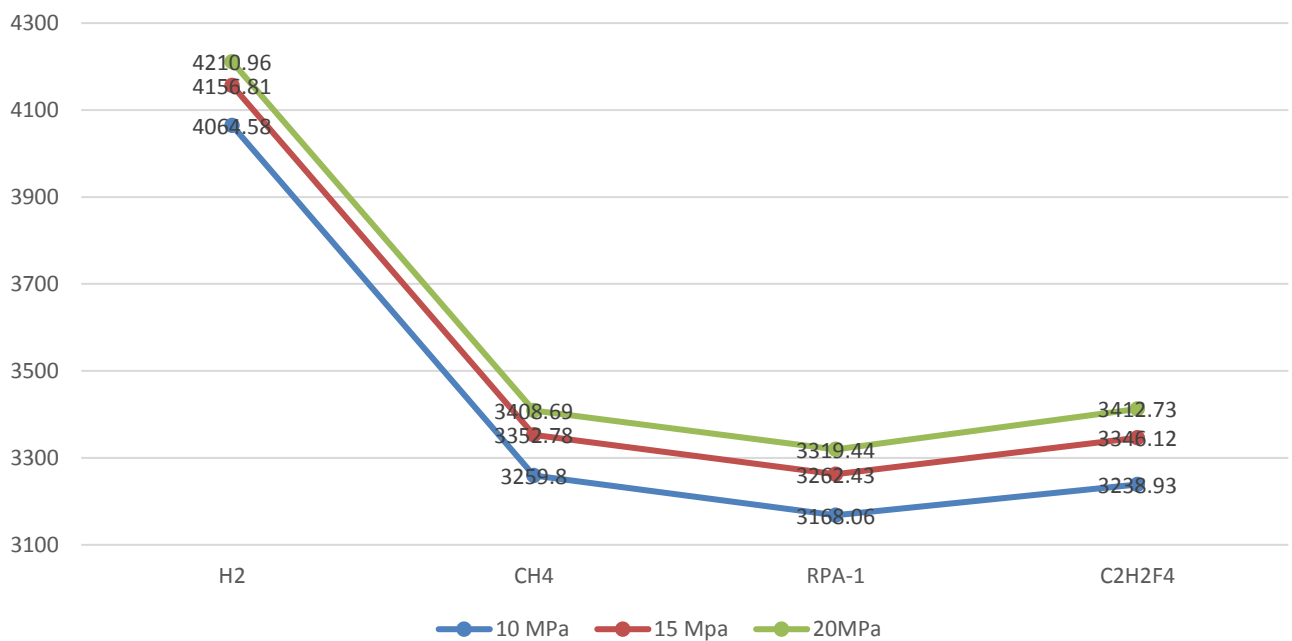
I_{sp} of fuels at different Chamber Pressure (Estimated)



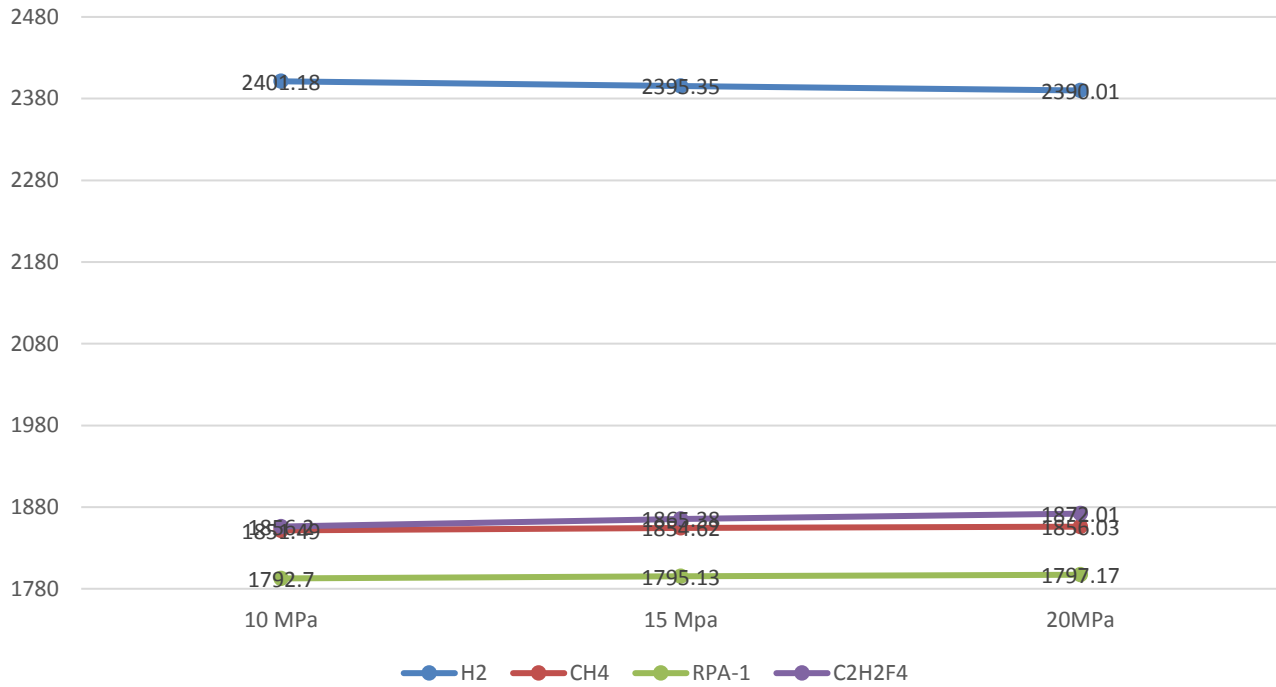
Effective Exhaust Velocity (m/s) of different fuels in vacuum (Ideal)



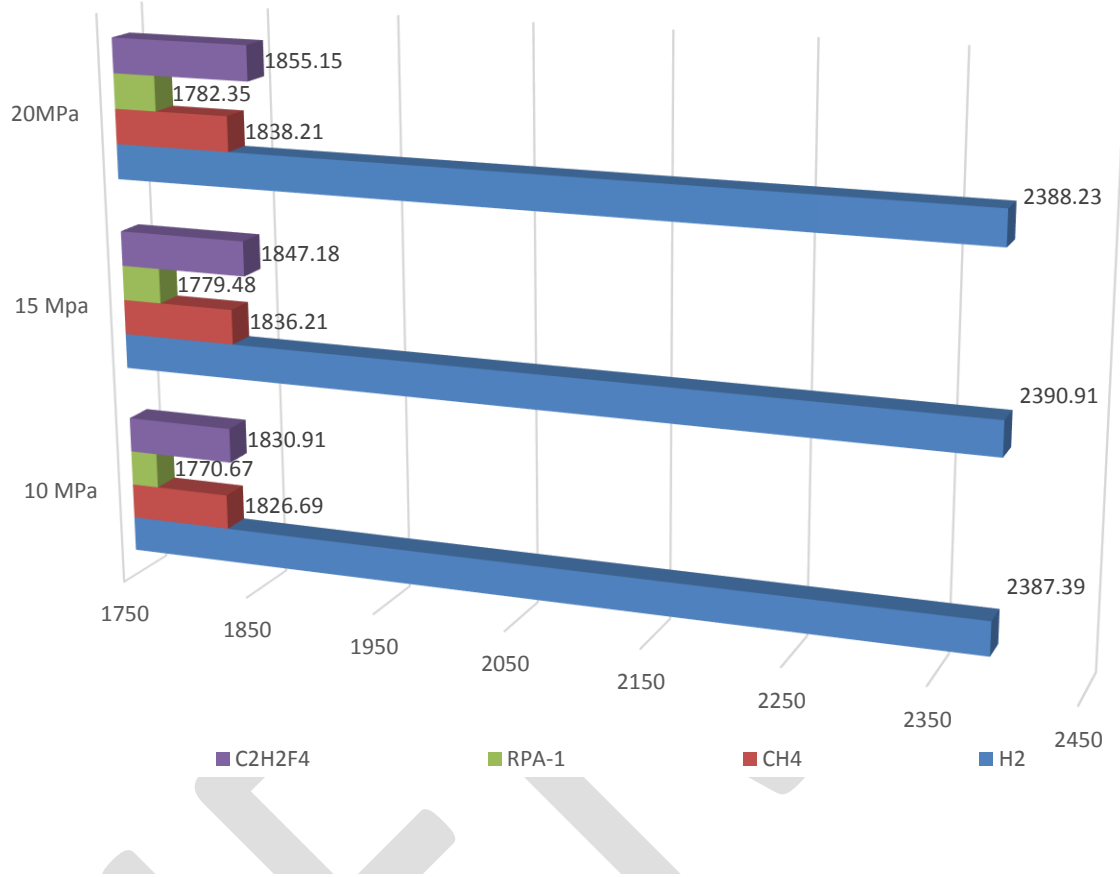
Effective Exhaust Velocity (m/s) of different fuels in vacuum (Estimated)



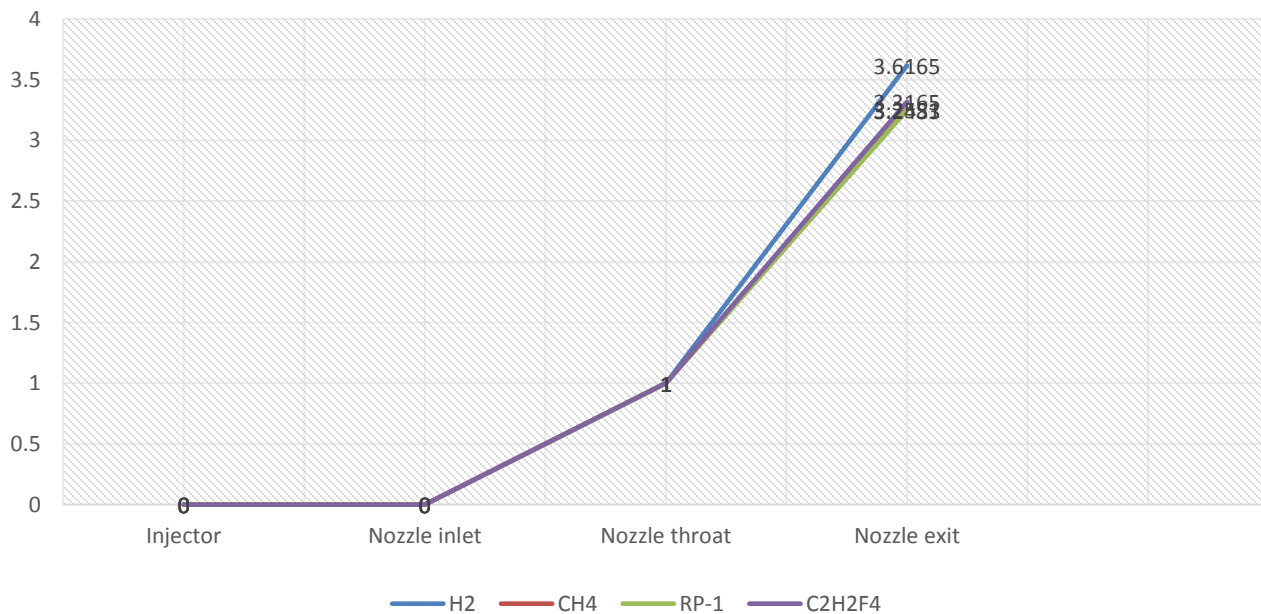
Characteristic Velocity (m/s) of fuels at different chamber pressure (Ideal)



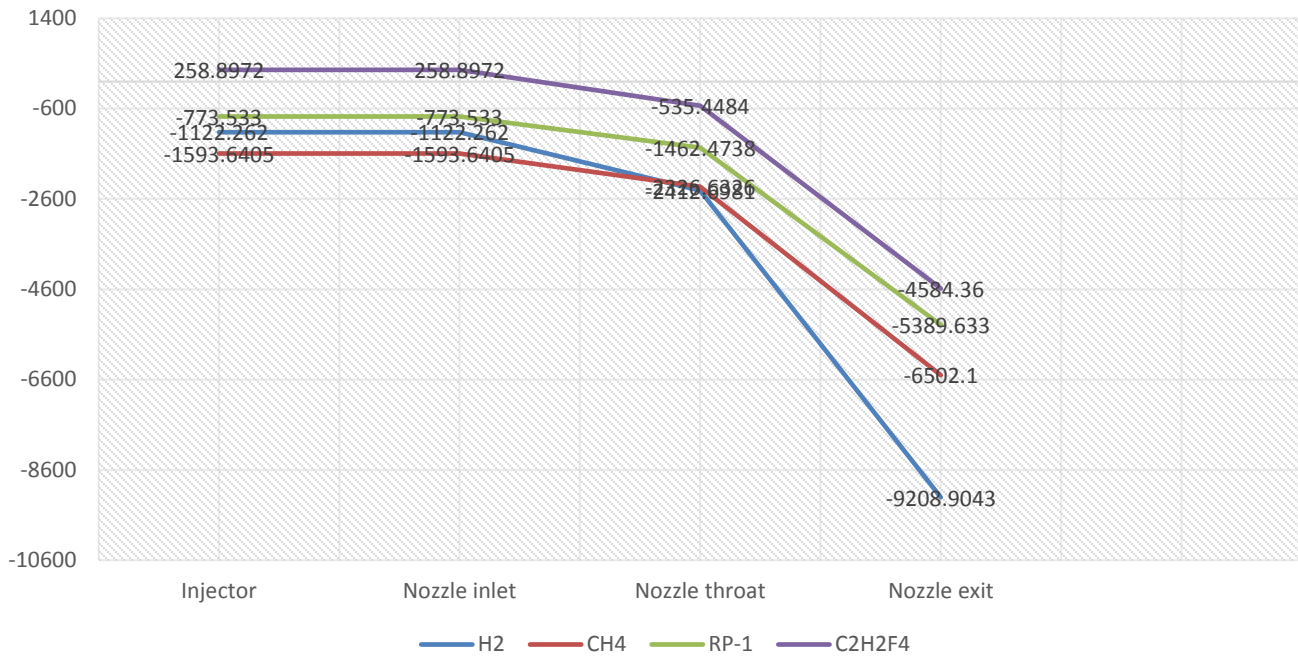
Characteristic Velocity (m/s) of fuels at different chamber pressure (Estimated)



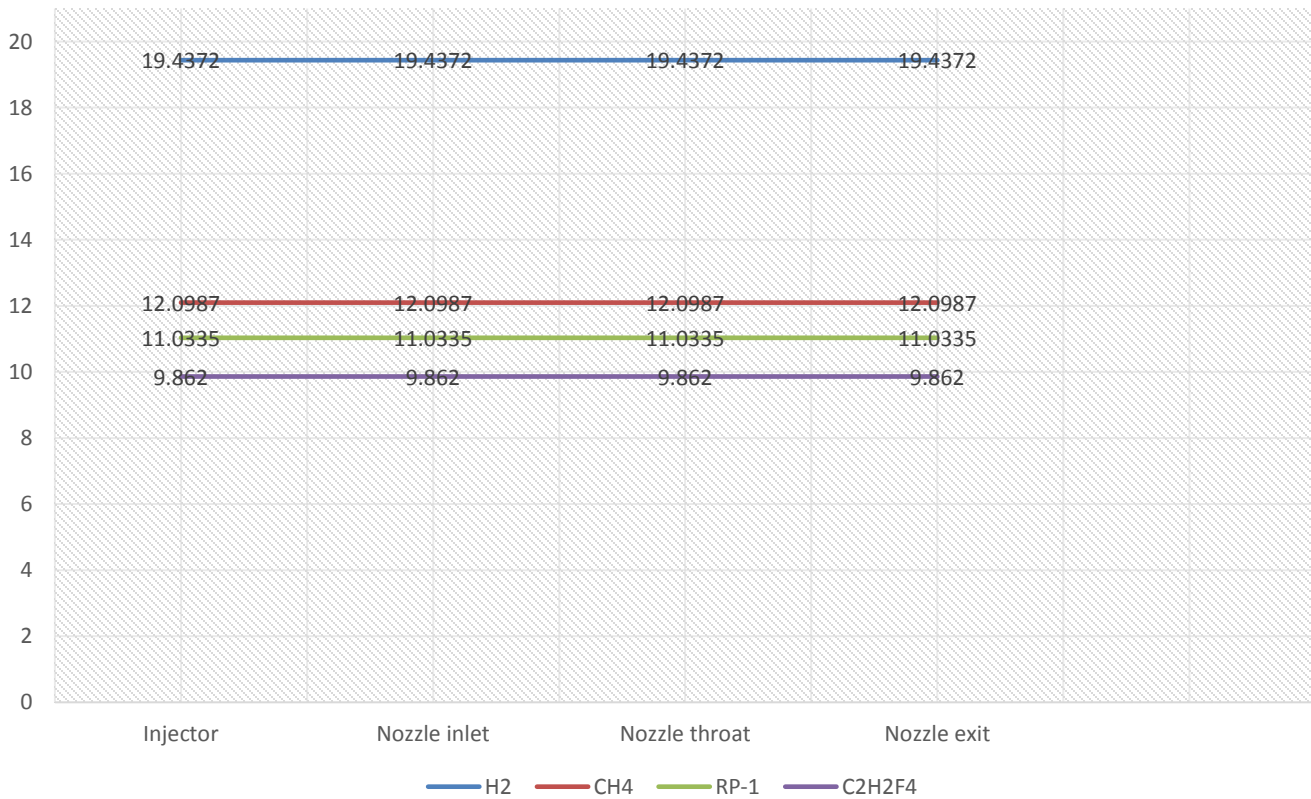
Mach No. Vs Station no



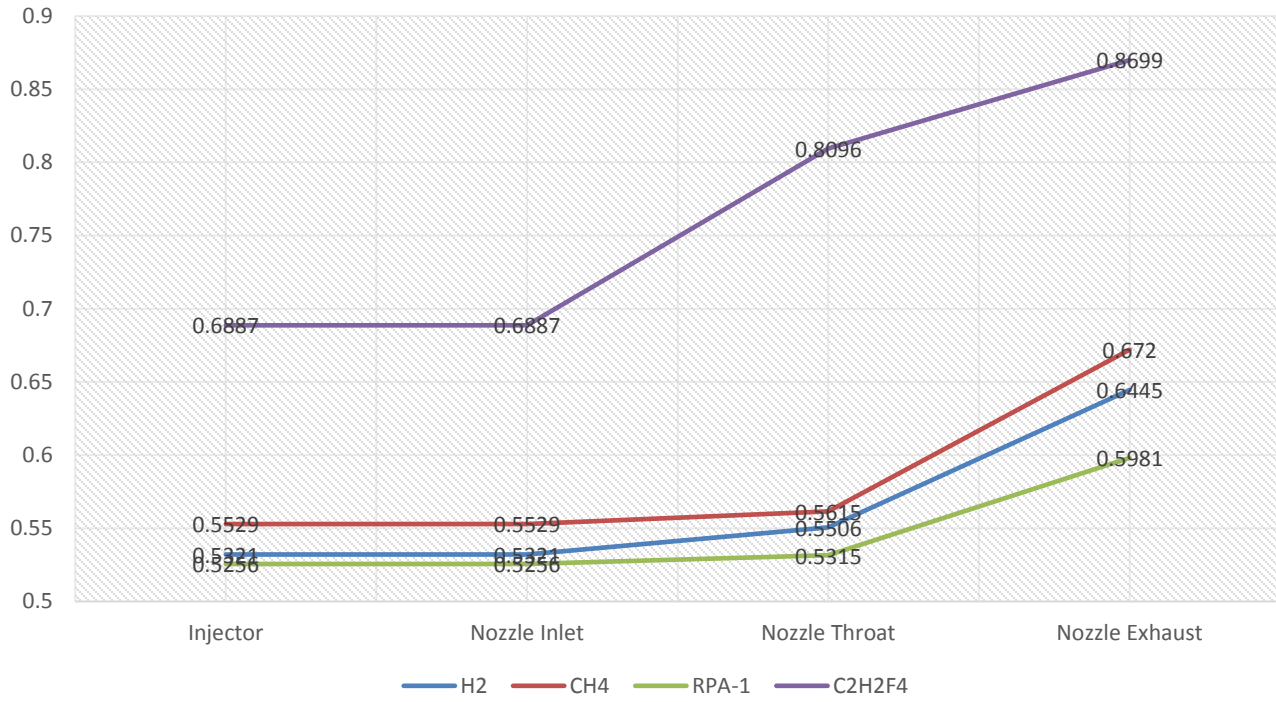
Enthalpy Vs Station no



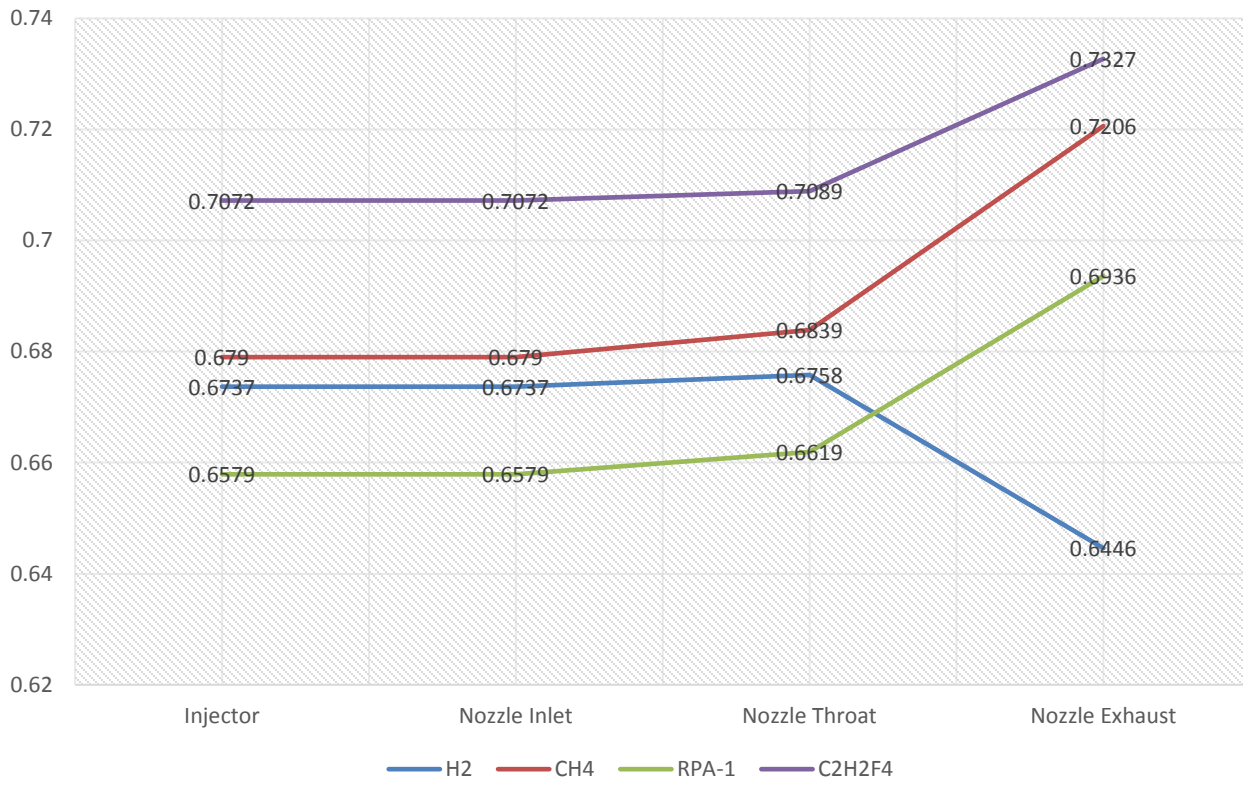
Entropy Vs Station no



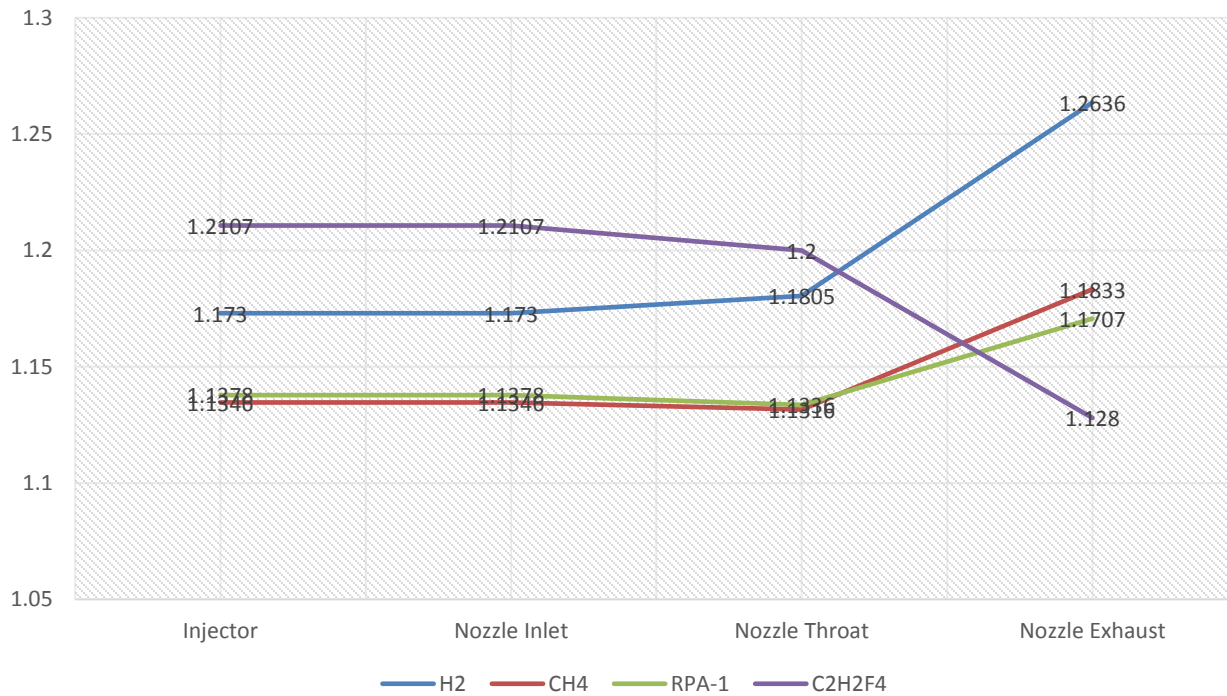
Prandtl no., effective flow Vs Station no.



Prandtl no., frozen flow Vs Station no



Isentropic Exponent Vs Station no



FUTURE SCOPE OF WORK

There are many different ways of analysing propellants with respect to different parameters hence widening the scope of the work to a vast extent. Further Analysis of the propellant can be made on the below mentioned areas:

- ❖ Multi-phase flow analysis
- ❖ Two phase flow
- ❖ Eulerian analysis
- ❖ Eulerian – Lagrangian analysis
- ❖ Chemical kinetics analysis
- ❖ Combustion characteristics analysis

CONCLUSION

The analyzation of species and their comparison with each other shows the difference in their thermodynamic properties. The deviation in the thrust coefficient of hydrogen, methane and RPA-1 is considerably large as compared to that of 1,1,1,2-tetrafluoroethane at 10MPa. As the chamber pressure increases, thrust coefficient of all the species increases simultaneously. Hydrogen has the highest Isp at 20MPa whereas RPA-1 has the lowest.

The effective exhaust velocity of the species is lower at estimated condition whereas in ideal condition hydrogen's velocity is way higher than other species. The deviation between 1,1,1,2-tetrafluoroethane and methane increases as the chamber pressure increases with increase in their characteristic velocity in ideal condition whereas the velocity increases very minutely in the case of the estimated condition.

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