

# Comparative Numerical Analysis of CD Nozzle with Hydrogen and Deuterium as Fuel

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## Abstract

*The Basic Rocket propulsion concept using the liquid Hydrogen as fuel and Liquid Oxygen as an oxidizer is re-modified with the liquid Deuterium, the isotope of hydrogen, to increase the thrust considerably and to increase the oxygen content on the atmosphere by nuclear interaction. The concept of Chemical propulsion and Molecular-level Expansion is integrated to increase the effective thrust and the fast-moving jet is made to interact with the atmospheric gasses to produce the desired effect so that the oxygen content is increased. This also stops the need for fossil fuels to explore space and emission of greenhouse gasses.*

**Keywords:** CD Nozzle, Computational fluid dynamics, deuterium-di-oxide, Hydrogen-di-oxide

## 1. Introduction

Till date many vehicles are either polluting the atmosphere or tuned with less amount of emission of the greenhouse gasses [1]. So, in an objective of developing a vehicle in rocket propulsion that could rectify the effects of the other polluting

vehicles, and produce a maximum thrust with the same size of fuel tanks, a change has to be made to the fuel that has more mass in a given volume and produce more thrust and higher range of specific impulse [2].

Deuterium  ${}_1\text{H}^2$  or  ${}_1\text{D}^2$ , also called DEUTERON, an isotope of the hydrogen has two nucleons (1 proton and 1 neutron), with an isotope mass of 2.014 amu [3,4]. The deuterium has a natural abundance of 0.0156% in the Earth [5]. This also can be produced artificially by using deuterium discharge tube. Deuterium is frequently represented by the chemical symbol D. Since it is an isotope of hydrogen with mass number 2, it is also represented by  ${}^2\text{H}$  [6].

Here is to compare the velocity vector of the CD Nozzle with  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$  with Computational Fluid Dynamics (CFD).

## 2. Computer simulation of nozzle

CFD is an engineering tool that assists experimentation. The following steps were performed in CFD of nozzle: Modeling, meshing, pre-processing, solution, post-processing.

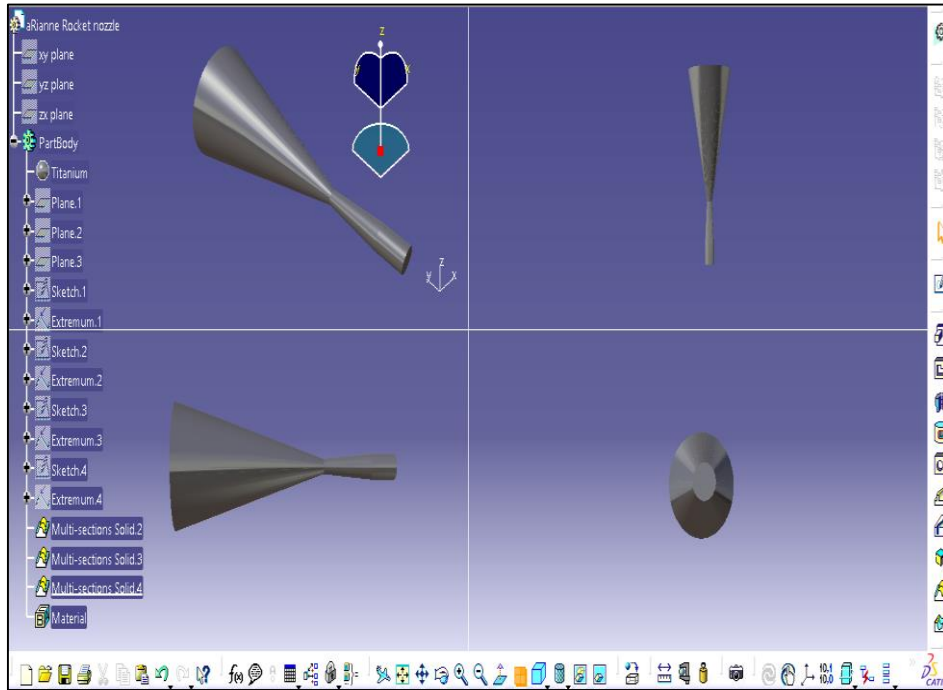
### 2.1 Modeling

The 2-Dimensional modeling of the nozzle was done using CATIA-V5 and file was saved in .stp format. The dimensions of the de Laval nozzle are presented in the Table 2.1 and the modeled CD Nozzle is given in Figure 2.1.

**Table 2.1 Nozzle dimensions**

S. No	DESIGN DATA	
	PARAMETERS	VALUE
1.	Area at throat	0.0127 m <sup>2</sup>
2.	Area at inlet	0.038 m <sup>2</sup>
3.	Area at exit	0.92 m <sup>2</sup>
4.	Radius at throat	0.064 m
5.	Radius at inlet	0.11 m
6.	Radius at exit	.54115 m

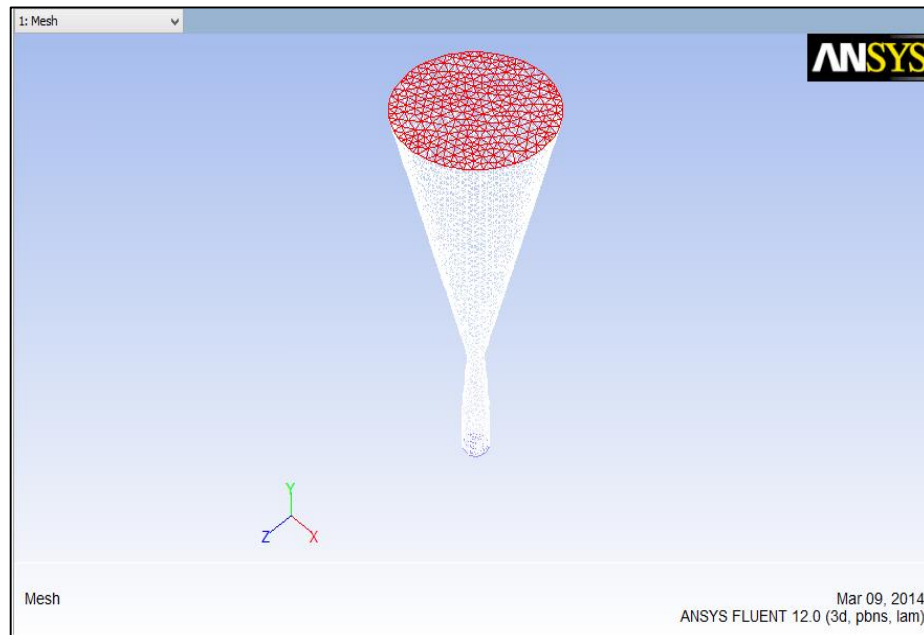
7.	Length convergent section	.640 m
8.	Length divergent section	2.020 m
9.	Angle of convergent section	15 deg
10.	Angle of divergent section	60 deg



**Figure 2.1 Nozzle 3 View Diagram**

## 2.2 Finite Element Analysis

The analyses were performed using Ansys. The model once imported from CATIA is then meshed with the Ansys AQWA mesh solver. In general task page the flow models are provided with pressure based and absolute velocity formulation. A gravity of 9.81 is defined in the Y-axis of the geometry. The Meshed CD Nozzle is shown in Figure 2.2



**Figure 2.2 Meshed Nozzle**

In models task page the Energy equation and the DES - Detached Eddy Simulation model is selected to select the RANS –Reynolds Averaged Navier Stroke Equation model as Spalart-Allmaras to simulate rocket Nozzle Flow.

In Materials task page the fluid is set as hydrogen-di-oxide/deuterium-di-oxide and the solid is set as Titanium as shown in Figure 2.3. Since the properties are function of Temperature the values are calculated for the Combustion chamber temperature of 3500 K with the following equations

Ratio of specific heats,

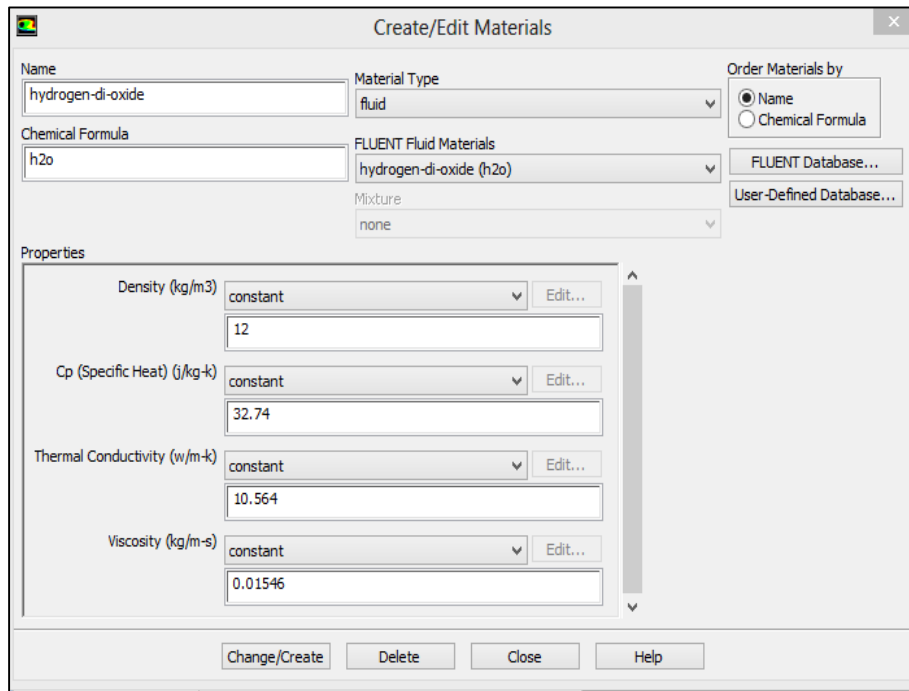
$$C_p = \gamma C_v \quad (1)$$

Thermal Conductivity,

$$K = K_0(1 + \beta T) \quad (2)$$

Dynamic viscosity,

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^n \quad (3)$$



**Figure 2.3 Creating Material**

### 2.2.1 Flow parameters used for fluids in the Analysis

The Flow parameters are listed in Table 2.2 given below.

**Table 2.2 Flow parameters for fluids**

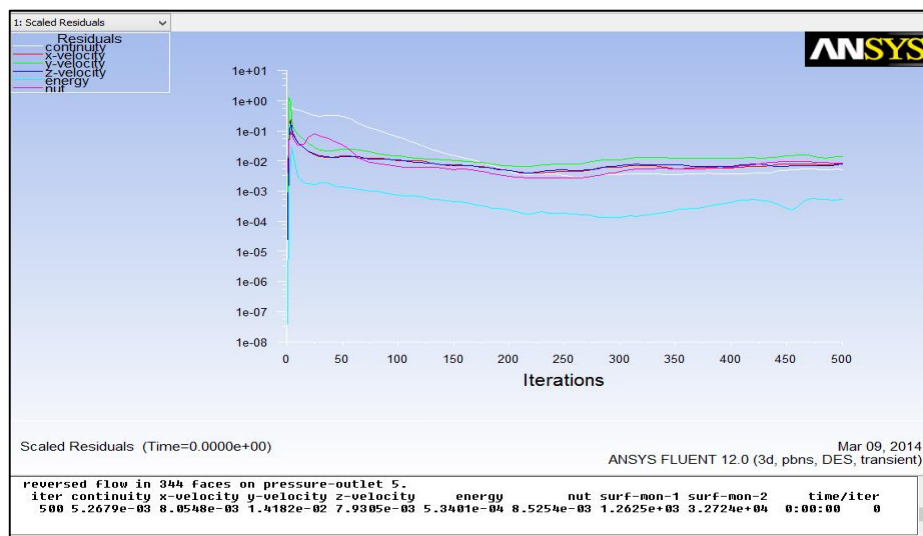
FLUID	MW	R	$\rho$	$C_v$	$C_p$	$\gamma$	K	$\mu$
<b>H<sub>2</sub>O</b>	18	461.88	12.3715	27.2833	32.74	1.2	10.564	0.01546
<b>D<sub>2</sub>O</b>	20	415.7	13.7461	12.7333	15.28	1.2	7.1	0.01286
<b>H<sub>2</sub></b>	2	4157	1.37461	3.25577	4.186	1.285	169456	0.0000499
<b>D<sub>2</sub></b>	4	2078.	2.74923	1.63333	2.1	1.285	127954	0.000111
<b>O<sub>2</sub></b>	16	519.6	10.9969	7.77777	10	1.285	23950	0.0000115

The cell zone conditions and the operating conditions are provided for the sea level conditions to operate at under expansion. The Boundary conditions are provided for the inlet-combustion chamber, nozzle wall and outlet-atmosphere as shown in Table 2.3

**Table 2.3 Boundary conditions**

Cell Zone	Boundary Condition	Velocity (m/s)	Pressure (Pa)	Temperature (K)
Combustion Chamber Inlet	Velocity-Inlet	800-1000 Variable	20000000	3500
Exit Area Sea-level	Pressure-Outlet	To be found	101325	288.88
Convergent and Divergent Section	Wall-Titanium	0	--	3500

Enable the required residuals and Set the Surface Monitors for Mass-flow rate and Exit-velocity to proceed to calculation. Initialize the solution with the injection velocity at the Velocity-inlet and then compute the flow from Velocity-inlet. Run the calculation for 500 Iteration to obtain a converged solution as in Figure 2.4



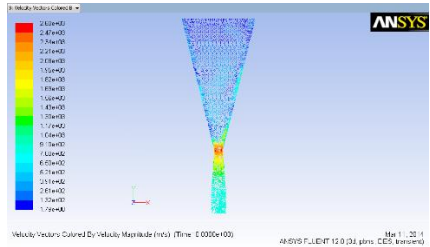
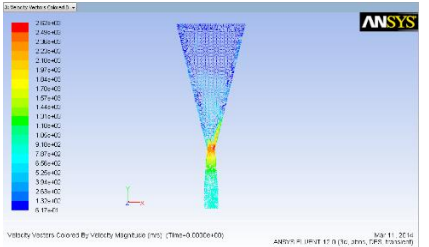
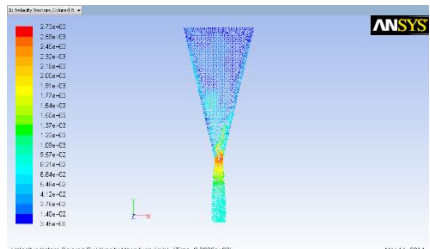
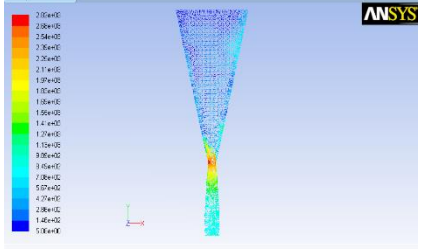
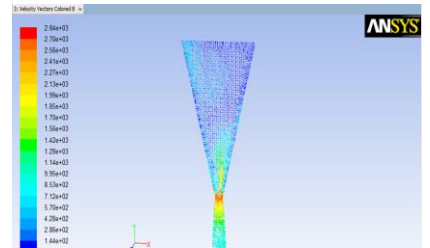
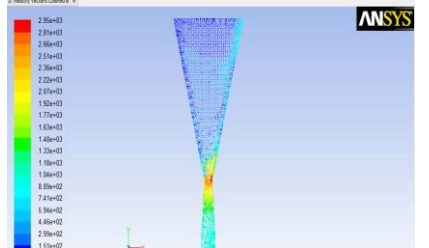
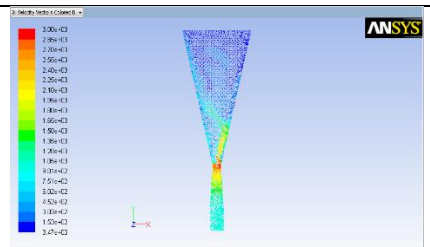
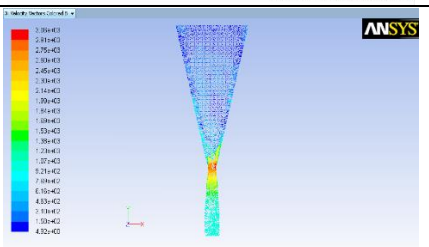
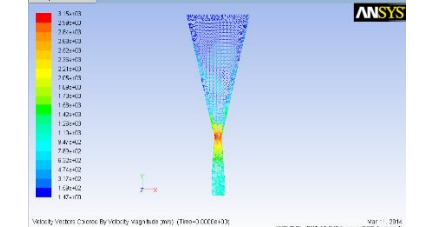
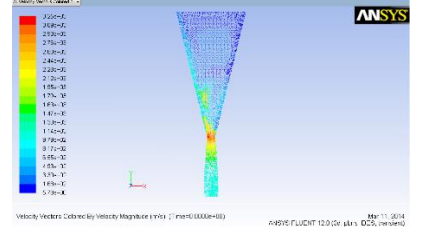
**Figure 2.4 Scaled Residuals**

### 3. Results and discussions

The Results are obtained as vectors and contour plots in the 2d form in XY-plane for Hydrogen as well as deuterium-di-oxide after 500 iteration of converging solution. The velocity is minimum at the inlet and goes on increasing till the nozzle exit. The velocity magnitude is Mach 1 at the throat section of the nozzle. This condition is known as choked flow condition. The velocity at the nozzle exit is 2600

m/sec for H<sub>2</sub>O and 2620m/sec for D<sub>2</sub>O. The obtained velocity vector contours are given in the Table 3.1

**Table 3.1 Velocity Vector Contours**

Velocity	H <sub>2</sub> O Velocity Vector	D <sub>2</sub> O Velocity Vector
800		
850		
900		
950		
1000		

#### 4. CONCLUSION

The results obtained by Computational Fluid Dynamics (CFD) for H<sub>2</sub>O and D<sub>2</sub>O clearly indicates the higher jet velocity for deuterium fuels. The values obtained from the analysis are listed in Table 4.1

**Table 4.1 Numerical Analysis of H<sub>2</sub>O and D<sub>2</sub>O**

S. No.	VELOCITY (m/s)	H <sub>2</sub> O	D <sub>2</sub> O
		JET VELOCITY (m/s)	JET VELOCITY (m/s)
1	800	2600	2620
2	850	2730	2820
3	900	2840	2950
4	950	3000	3060
5	1000	3150	3250

From the results it is evident that, deuterium is considered to have an advantage of higher thrust on rocket than the conventional hydrogen, both in natural and cryogenic state and hydrogen can be replaced as a better fuel with deuterium. As present work the analysis has been done in a numerical way, with the both H<sub>2</sub> and D<sub>2</sub> fuels and a feasible high thrust rocket model is proposed. Continuous usage of the deuterium rockets restores the oxygen content from nitrogen transformation, and in turn reduces carbon content by transforming it to nitrogen for compensation.

#### 5. References

- [1] Harrison, R. M., Masiol, M., & Vardoulakis, S., "Civil aviation, air pollution and human health", *Environmental Research Letters*, vol.10, no. 4, (2015).
- [2] Dessens, O., Anger, A., Barker, T., & Pyle, J., "Effects of decarbonizing international shipping and aviation on climate mitigation and air pollution. *Environmental Science & Policy*", vol. 44, (2014), pp. 1–10.



[3] Epstein, R. I., Lattimer, J. M., & Schramm, D. N., “The origin of deuterium. *Nature*”, vol. 263, no. 5574, **(1976)**, pp. 198–202.

[4] Engen, J. R., Botzanowski, T., Peterle, D., Georgescauld, F., & Wales, T. E., “Developments in Hydrogen/Deuterium Exchange Mass Spectrometry”, *Analytical Chemistry*, vol. 93, no. 1, **(2020)**, pp. 567-582.

[5] Pirali, T., Serafini, M., Cargnin, S., & Genazzani, A. A., “Applications of deuterium in medicinal chemistry”, *Journal of Medicinal Chemistry*, vol. 62, no. 11 **(2019)**, pp. 5276-5297.

[6] Rely Victoria Petrescu, “Sustainable Energy for Aerospace Vessels”, *Journal of Aircraft and Spacecraft Technology*, vol. 1 no. 4, **(2017)**, pp. 234.240