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CFD simulation with analytical verification of discharging of nitrogen and helium from a high-pressure gas vessel

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Abstract. Many applications and industrial processes may necessitate the storage of large amounts of gases at high pressures. These compressed gases could be extremely dangerous if unintentionally released. since they could be poisonous or combustible when mixed with air. This research seeks to create a CFD model and undertake an analytical investigation of the process of de-pressurization of high-pressure gas from a vessel. The vessel to be studied is used in a pneumatic power system used to operate the control surface of a flying vehicle. The study involved two working fluids (nitrogen and helium). The discharging process is considered as a typical mass and heat transfer problem solved analytically by adopting The First Law of Thermodynamics to an unsteady flow control volume and simulated by employing transient flow analysis to the CFD model. The research was carried out on 440 bars (absolute pressure) of pressurized gas vessels. Working gases for the study included nitrogen and helium. Analytical solution results for the two different gases have been compared with the CFD simulation results to assess the CFD model's accuracy. A good match is achieved when the gas temperature, pressure, density, and outlet mass flow rate variations are compared. The results demonstrated a good match between the CFD and analytical data, proving the validity of the CFD model.

1 Introduction

Currently, compressed gas is employed in a wide range of applications, including power plants, oil refineries, automotive, aerospace industries, Chemical Manufacturing, Glass Manufacturing, General Manufacturing, Hospitals/Medical, Pharmaceuticals, Electronics, Food and Beverage, Wood Products, and many more. In automobile gas tanks, High-pressure compressed hydrogen is stored and used as fuel. While power plants and oil refineries facilities employ compressed natural gas and air. In the defense industries and aerospace, Pure gas with maximum compressed power is critical for weapon and aircraft manufacturers. for example launch vehicles use different high-pressure gases for different purposes, gaseous helium is used for tank pressurization, hydrogen gas is used in the start-up system for the engine while high-pressure nitrogen is used in the auxiliary propulsion system. for the remaining applicants Compressed gas is mostly employed in tool powering, actuators, and controls.

In this research, a pneumatic power system, shown in Figure1, used to control a flying vehicle was to be simulated using the CFD techniques. This work seeks to partially verify the whole system model and verify the method used in the simulation. The model was used to compute the vessel's outlet mass flow rate, temperature, and discharging time which might be an indication

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of control time during the discharging process. A comparison between nitrogen and helium shall be attempted to distinguish the performance between these two gases.

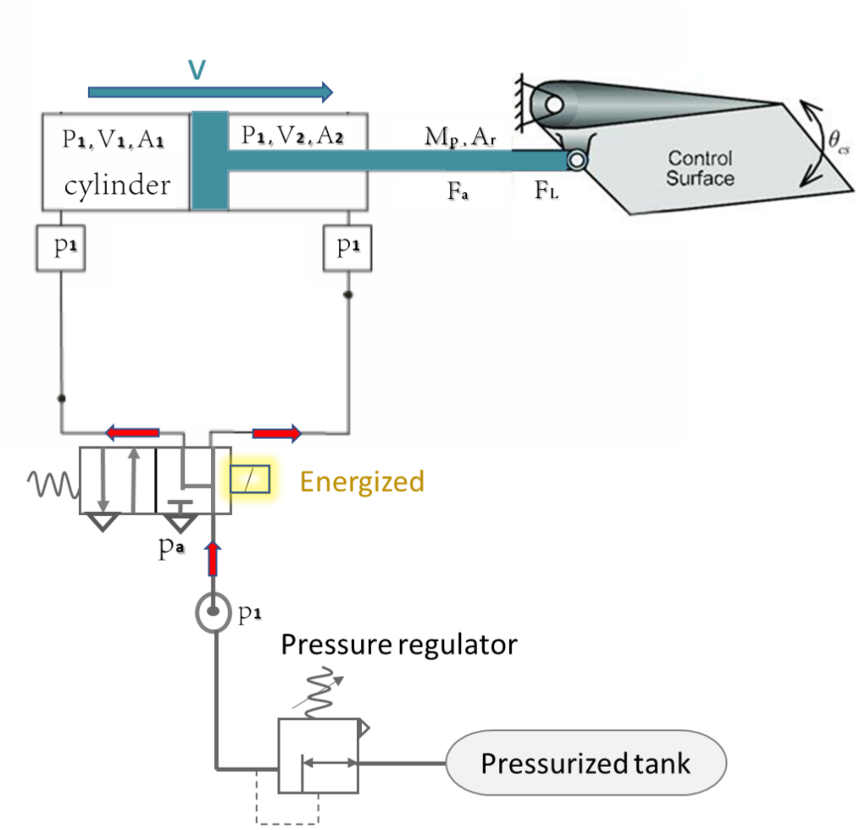


Figure 1. pneumatic circuit used to drive the control surface.

1.1 *Literature survey.*

Numerical simulation and an analytical solution have both been used to study the discharging of a pressurized bottle. Discharging a pressurized bottle entails releasing gas from the bottle through a controlling valve or an orifice. Several factors influence fluid flow, including the pressure inside the bottle, the size and shape of the orifice, and the fluid's properties.

Numerous previous research has employed numerical simulation and experimental investigations to study the charging and discharging process from pressurized bottles. The common kinds of literature have focused on filling high-pressure reservoirs, but there is not much research on the process of de-pressurizing gas bottles. This work attempts to provide a better understanding of the flow physics of tank discharge.

There are different methods followed for solving such a problem. Some researchers considered analytical solutions validated with experimental work such as a previous study by Winters et al[1] which included an examination of noncondensing gas flow and heat transfer during the venting of tanks. The study provided an analysis solution validated with experimental work. The analysis solution implemented a Single control volume with correlations for heat transfer using NETFLOW analysis code coupled with code-coupling, FUEGO at the exit for Multi-dimensional analysis to predict temperature and pressure. Johnston and Dwyer [2] used Schlieren imaging to study the structure of discharged FLOW from a high-pressure gas reservoir and conducted numerical solutions that agreed with the experimental data. where G. Artingstall [3] Studied the gas discharging process from a high-pressure container analytically by solving the continuity equation and the equation of state and considered the mixing with the atmosphere during the process and the buoyancy-driven flows that cause the gas to be discharged from the container.On other hand, Dhaouet al [4] studied the discharge operation from metal–hydrogen tank using the mathematical model provided by Jemni et al[4] which is based on (energy equation and continuity equation) then the model was validated with experiential work.

Some other research considered CFD simulation validated with experimental work such as a study by Dicken and Merida [[5],[6]] researched how temperature distribution in high-pressure hydrogen tanks is affected by initial mass and filling time during refueling considering axisymmetric flow for the numerical study neglecting the effects of buoyancy and gravitational forces which appeared to be unsuitable for longer filling times. Suryan et al[[7],[8]]used the k-ω turbulence model to solve Three dimensional, compressible, unsteady Navier Stokes equations incorporating real gas properties to accurately predict the gaseous hydrogen's dynamic behavior while filling a tank with high pressure.

Hasalova et al[9] used a 2D steady model in ANSYS CFX 17.2 studying the CNG flow characteristics from the fuel tank through 3mm orifice neglecting compressibility factor change and Heat transfer effects. The SST k-ω turbulence model was considered for the simulation. while Reynolds and Kays [10] concerned with heat transfer accompanying gases during charging or discharging from vessels, utilizing the correlations for natural convection.

D. Melideo et al [11] investigated the discharge of hydrogen cylinders at two distinct mass flow rates and verified a CFD model created using experimental data.

some researchers considered the use of helium or nitrogen for the study such Clark [12] studied the rapid discharge of nitrogen and helium from a vessel for turbulent and laminar flow experimentally.

Charton et al[13]. studied the discharge of deuterium and helium from cylindrical and spherical vessels to a vacuum chamber through a long tube for laminar and turbulent conditions.

Woodfield et al[14]. studied the filling and discharging of cylinders with nitrogen, hydrogen, and argon gas. Heat transfer to and from the discharging and charging gas was measured using a spatially averaged transient thermocouple and heat flux measurements.

Although there are different theoretical solutions in the literature, there is no study that described the solution to such a problem by adopting The First Law of Thermodynamics to an unsteady flow control volume. The purpose of the study is to develop a mathematical model that can predict the evolution of temperature, density, pressure, and mass flow rate as a gas bottle depressurizes for both helium and nitrogen by adopting The First Law of Thermodynamics to an unsteady flow control volume. Then using the model results to verify the CFD model. A comparison between helium and nitrogen shall be presented to indicate which fluid performs better during the operation of the pneumatic system shown in Figure 1.

2 Numerical Simulation(Computational Model and Boundary Conditions).

The two-dimensional model of the vessel is shown in Figure 2, which is composed of the exit and the fluid domain. Figure 3 shows the mesh model of the vessel. As the vessel model is symmetrical, the computational domain was made to simulate only half of the model. A structured grid was used. Two fluid mediums were tried inside the vessel (Helium and Nitrogen) with a pressure of 440 bar patched as the initial Pressure for the fluid domain. An outlet Pressure P_2 of 1atm was chosen as a boundary condition at the exit. The center axis(x-axis) was set as symmetry. Transient-state solvers with the second-order upwind scheme were adopted. Pressure-based realizable k-ϵ turbulence model was used since it gave a better accuracy in the study ([15] ,[16] , [17]).

To guarantee the precision of the numerical approach used in this study. Two different steps using Helium as the working fluid were performed before the final simulation. The first step was concerned with the choice of the suitable time step size used in the simulation. As shown in Table 1 for the range of chocked flow (the sonic speed at exit) and un-choked flow different time steps were tried to calculate the time taken for the vessel pressure to decrease from an initial value $P_o = 440$ bar to a critical value $P_{cr} = 2.08016$ bar(choked flow regime) and to calculate time to decrease from that critical value to the atmospheric value (P_2 =1.01325 bar)(un-choked flow regime). From Table 1 it can be seen that below a time step size of (1.86E-05 sec), there is no change in the time taken to reach the critical pressure P_{cr} or to reach the atmospheric pressure P_2. so, a time step size of (1.86E-05 sec) was used for the simulation. The second step was to perform a Grid-independence study using the predetermined time step size (1.86E-05 sec). Table 2 shows that the depressurization rate in the vessel changes with different grid numbers .and it can be found that the mesh size (0.1 mm) with a grid number of 284400 is a suitable choice. so it can be selected to ensure the accuracy and efficiency of the simulation results.

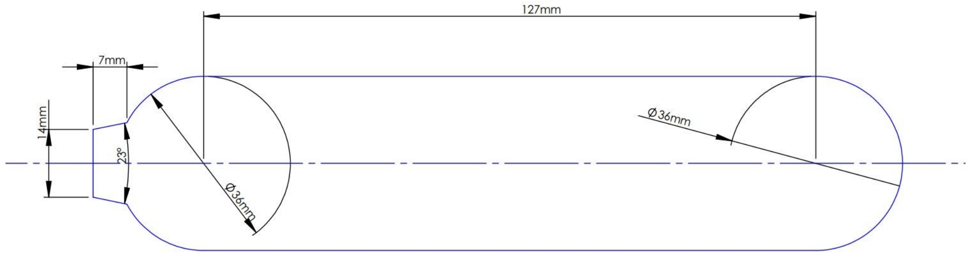


Figure 2. 2-D geometrical dimension of the vessel.

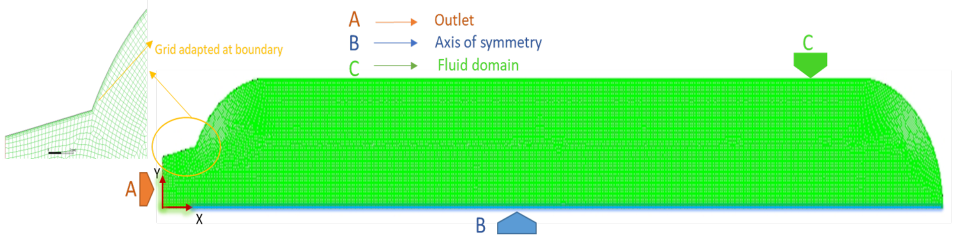


Figure 3. The vessel's mesh model.

3 Mathematical model (analytical solution).

In order to verify the CFD simulation, an analytical solution was conducted on the depressurization of gaseous helium and nitrogen from a storage vessel using Matlab to solve the first law of thermodynamics in the transient state using the same conditions and geometric parameters used in the CFD simulation listed in Table 3.

3.1 Governing Equations.

Gaseous helium (or nitrogen) is stored in the storage vessel at very high pressure. Regarding the storage conditions including temperature, pressure, and compressibility factor, the initial

Table 1. simulation with different time step sizes.

Time step size [sec]	$Time^1$ to reach P_{cr} [ms]	$Time^2$ to reach P_2 [ms]
1.86E-04	9.8885	15.71
9.30E-05	9.6549	12.857
4.66E-05	9.546	12.711
1.86E-05	9.537	12.695
1.33E-05	9.537	12.679
9.30E-06	9.537	12.6828

^1Time taken to decrease from P_o to P_{cr} (choked flow only).
^2Time taken to decrease from P_o to P_2 (choked flow + unchoked flow).

Table 2.

mesh size (mm)	Grid number (10ˆ3)	$Time^1$ to reach P_{cr} [ms]	δ (%)	$Time^2$ to reach P_2 [ms]	δ (%)
1	3.6	9.3169	6.83	12.3776	7.97
0.8	5.5	9.4443	5.56	12.540	6.77
0.6	9.3	9.6125	3.87	12.7324	5.34
0.4	19.5	9.7347	2.65	12.8772	4.26
0.3	33.9	9.8036	1.96	12.9514	3.71
0.2	73	9.8689	1.31	13.0259	3.15
0.1	284.8	9.92852	0.71	13.1045	2.57
0.08	460.6	9.93042	0.70	13.1075	2.55
0.06	730.5	9.93082	0.69	13.1082	2.54

[δ %] = [Error %] = 100 × (analytical solution result -CFD's result)/ analytical solution result.

Table 3. different specifications used in the solution.

parameter	value
Volume of gas bottle	0.15 Litres
Bottle exit diameter	14 mm
Storage temperature	300 k
Storage pressure	440 bar
Fluid 1	He with γ = 1.667 and R= 2076.9 J/kg.K
Fluid 2	N_2 with γ =1.4 and R=296.8 J/kg.K

storage mass (m_o) is estimated. And it is possible to estimate the instantaneous mass after discharging a specific mass of gas. The schematic for the processes of mass transfer during the release of stored gas from a vessel is shown in Figure 4. The study is performed using a lumped model of a single control volume. That approach is considered valid. Since the pressures in the vessel are almost uniform in the whole domain during the entire transient discharge. As the exit area is small in comparison to the vessel diameter. Both pressure and temperature were predicted using the single control volume analysis. Pressure decay and gas temperature are estimated and compared with the CFD simulation.

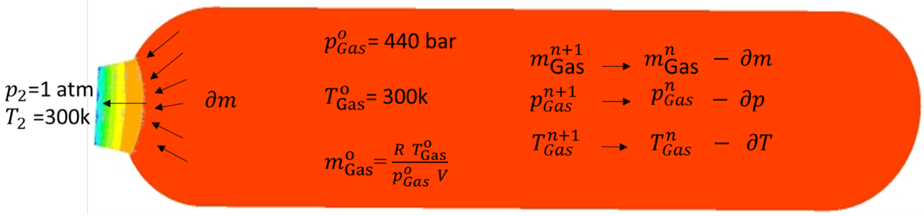


Figure 4. Schematic diagram represents mass transfer during bottle de-pressurization.

Assumptions:

- Lumped model of a single control volume.
- Homogeneous gas properties in the vessel.
- ρ (density), T (temperature) remains constant during Δt.
- Gas (helium or nitrogen) obeying perfect gas law.

The First Law of Thermodynamics is applied to the unsteady single control volume. The equations can be discretized by using the forward difference formula as the problem can be considered as time marching in the sense.

$$\dot{Q} - \dot{W} = \frac{dE_{\text{Gas}}}{dt} + \dot{m}_{\text{out}} \left(h_{\text{out}} + \frac{1}{2}V_{\text{out}}^2 + gz_{\text{out}} \right) - \dot{m}_i \left(h_i + \frac{1}{2}V_i^2 + gz_i \right) \tag{1}$$

$$\frac{dE_{\text{Gas}}}{dt} = \frac{m^{n+1}_{\text{Gas}} \left(u^{n+1}_{\text{Gas}} + gz^{n+1} \right) - m^{n}_{\text{Gas}} \left(u^{n}_{\text{Gas}} + gz^{n} \right)}{\Delta t} \tag{2}$$

$$\frac{dm_{\text{Gas}}}{dt} = \dot{m}_{\text{in}} - \dot{m}_{\text{out}} \tag{3}$$

Boundary conditions are:

- $\dot{m}_{\text{in}} = 0$ (no inflow).
- $\dot{W} = 0$ (as there is no moving boundary work involved).
- $\dot{Q}$= heat transferred= 0.

$$m^{\circ}_{\text{Gas}} = \frac{RT^{\circ}_{Gas}}{p^{\circ}_{Gas}V} \tag{4}$$

$$u^{\circ}_{\text{Gas}} = c_v T^{\circ}_{\text{Gas}} \tag{5}$$

$$\frac{m^{n+1}_{\text{Gas}} - m^{n}_{\text{Gas}}}{\Delta t} = -\dot{m}^{n}_{out} \tag{6}$$

$$m^{n+1}_{\text{Gas}} = m^{n}_{\text{Gas}} - \dot{m}_{out}\Delta t \tag{7}$$

$$\frac{\left(m^{n}_{Gas} - \dot{m}_{\text{out}}\ \Delta t\right) u^{n+1}_{Gas} - m^{n}_{Gas} u^{n}_{Gas}}{\Delta t} = -\dot{m}_{\text{out}} \left(h_{\text{out}} + \frac{1}{2} V_{\text{out}}{}^2 \right) \tag{8}$$

$$u^{n+1}_{\text{Gas}} = \frac{m^{n}_{\text{Gas}}\ u^{n}_{\text{Gas}} - \dot{m}^{n}_{\text{out}}\ \Delta t \left(h^{n}_{\text{out}} + \frac{1}{2} V^{n}_{\text{out}}{}^2 \right)}{\left(m^{n}_{\text{Gas}} - \dot{m}_{\text{out}}\ \Delta t \right)} \tag{9}$$

$$\dot{m}_{\text{out}}^{n} = A_e \rho_e V_{\text{out}}^{\text{n}} \tag{10}$$

$$V_{\text{out}}^{\text{n}} = \text{M}_{\text{e}}^{n} \sqrt{\gamma R T_e^n} \tag{11}$$

$$h_{\text{out}}^{n} = c_p T_e^n \tag{12}$$

We can now calculate u_{Gas}^{n+1} and from this T_{Gas}^{n+1}.

$$T_{Gas}^{n+1} = \frac{u_{Gas}^{n+1}}{c_v} \tag{13}$$

Using m_{Gas}^{n+1} and T_e^{n+1} to calculate p^{n+1}.

$$p_{Gas}^{n+1} = \frac{m_{Gas}^{n+1} R T_{Gas}^{n+1}}{V} \tag{14}$$

If the pressure in the vessel (p_{Gas}^n)is above some critical value (P_{cr})that given by:

$$p_{cr} = \left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}} p_2 \tag{15}$$

where p_2 is the atmospheric(back) pressure. It's found that flow is choked which means that the flow speed at the exit will be sonic (M_e^n=1). And hence the temperature at the exit (T_e^n) can be calculated as:

$$Y = \left(\frac{2}{\gamma+1}\right) \tag{16}$$

$$T_e^n = Y T_{Gas}^n \tag{17}$$

When the choking phenomena (sonic-flow regime) breaks down and the pressure in the vessel (p_{Gas}^n)is lower than the critical value(p_{Gas}^n<p_{cr}), the gas will discharge from the vessel at subsonic velocities. Then the temperature (T_e^n) and the Mach number (M_e^n) at the exit can be calculated as:

$$Y = \left(\frac{p_2}{p_{Gas}^n}\right)^{\frac{\gamma-1}{\gamma}} \tag{18}$$

$$T_e^n = Y T_{Gas}^n \tag{19}$$

$$\mathbf{M}_{\text{e}}^{n} = \sqrt{\left(\left(\frac{p_2}{p_{Gas}^n}\right)^{\frac{1-\gamma}{\gamma}} - 1\right)\left(\frac{2}{\gamma-1}\right)} \tag{20}$$

3.2 Algorithm followed for the Code.

The code was written in Matlab, to calculate the mass flow rate out of the vessel and the time taken to empty the vessel by calculating pressure and temperature decrease with time; using the above mathematical formulation equations and following the algorithm shown in Figure 5.

3.3 Verification of numerical model using an analytical solution.

In this section results from the numerical analysis and the analytical solutions are presented. Comparisons are made with results from the analytical and the numerical model.

Figures(6 ,7 , 8 , 9) demonstrate the comparison of the results of the CFD model and the analytical solution for pressure, temperature, density, and the mass flow rate out of the vessel respectively. The results show good agreement between the CFD model and the analytical solution.

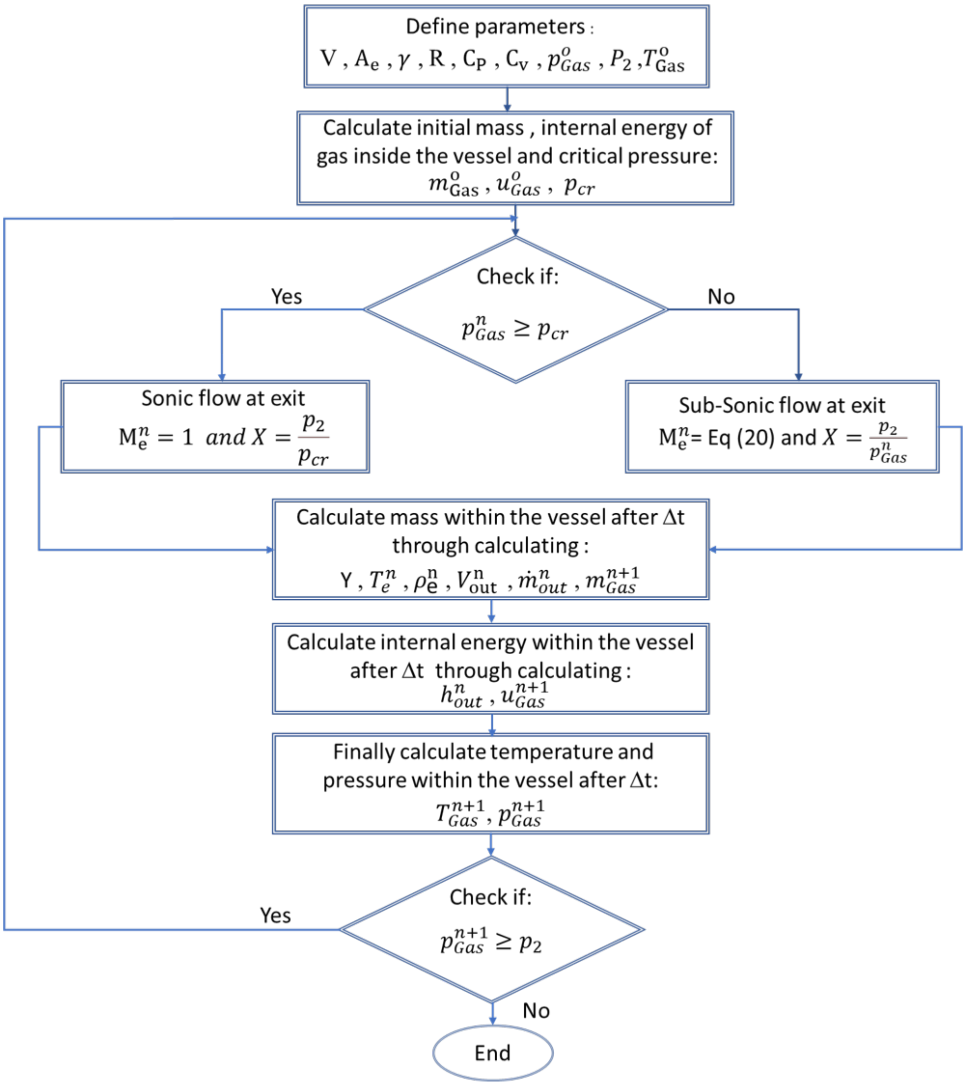
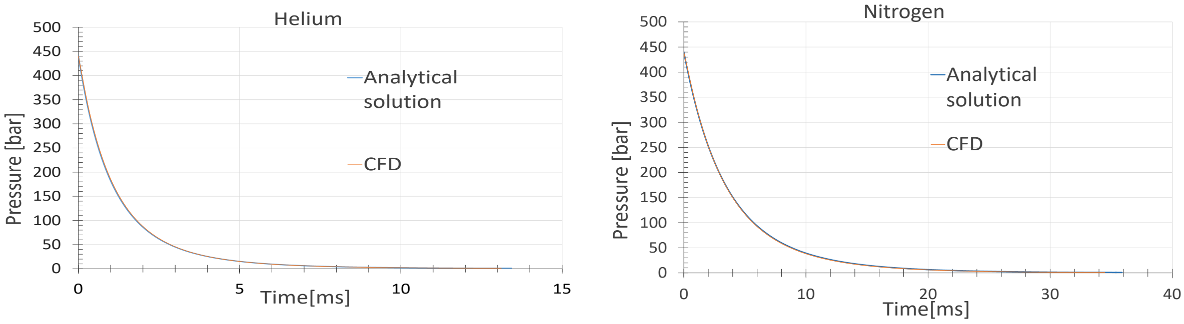


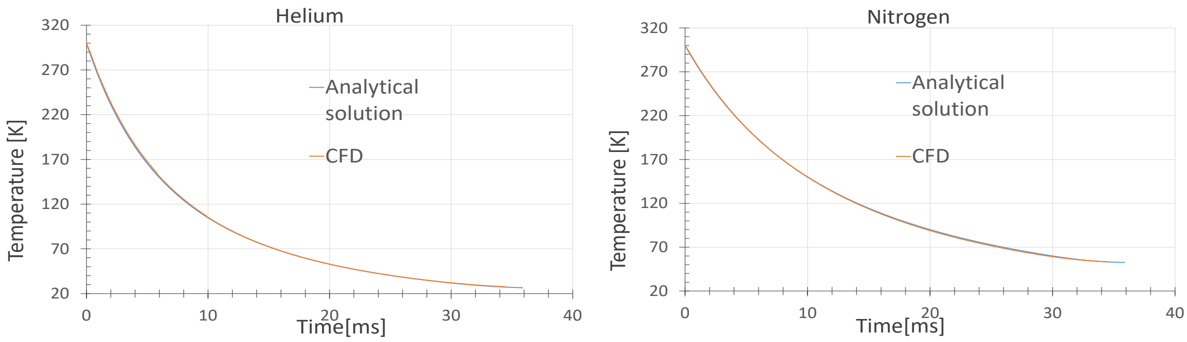
Figure 5. Schematic diagram represents mass transfer during bottle de-pressurization.



(a) Helium

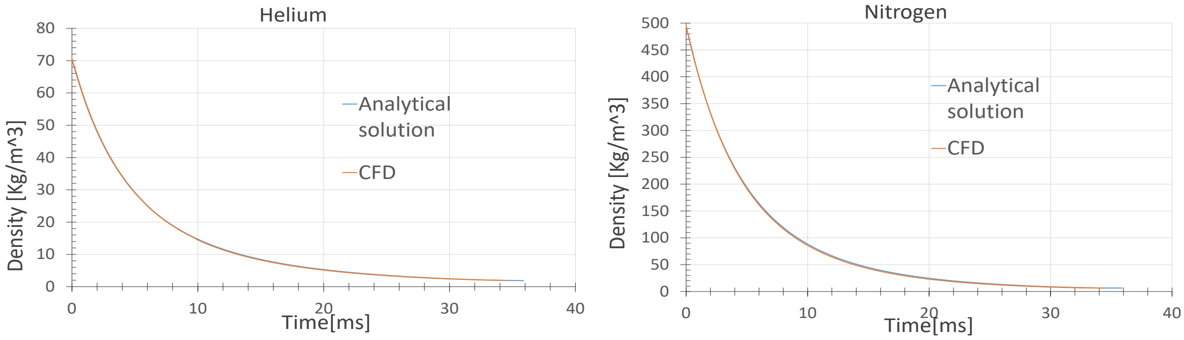
(b) Nitrogen

Figure 6. Gas Pressure evolution Comparison between CFD and analytical solution for both helium and nitrogen.



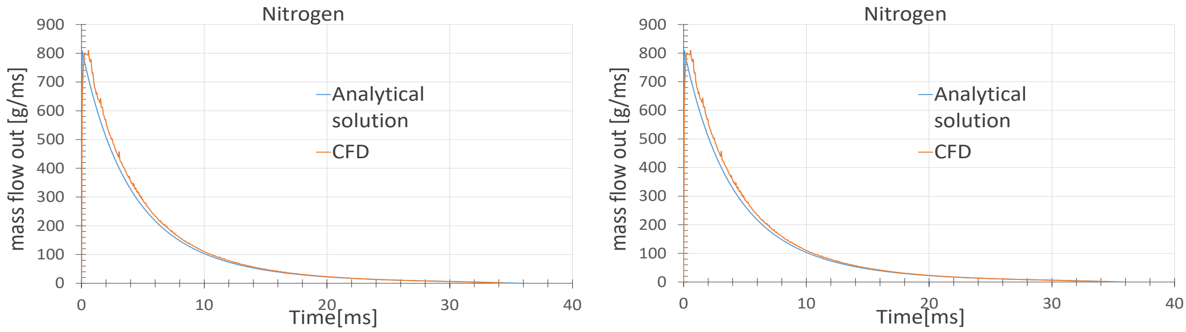
(a) Helium (b) Nitrogen

Figure 7. Gas Temperature evolution Comparison between CFD and analytical solution for both helium and nitrogen.



(a) Helium (b) Nitrogen

Figure 8. Gas Density evolution Comparison between CFD and analytical solution for both helium and nitrogen.



(a) Helium (b) Nitrogen

Figure 9. Mass flow rate out Comparison between CFD and analytical solution.

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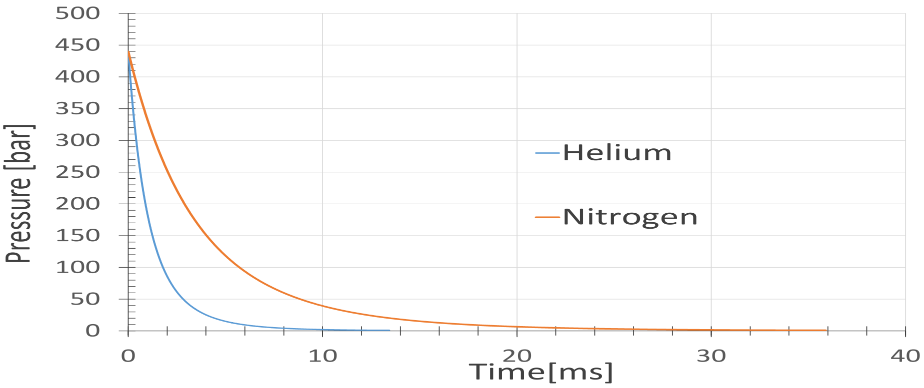

Figure 10. Comparison of Gas Pressure Evaluation Between Helium and Nitrogen.

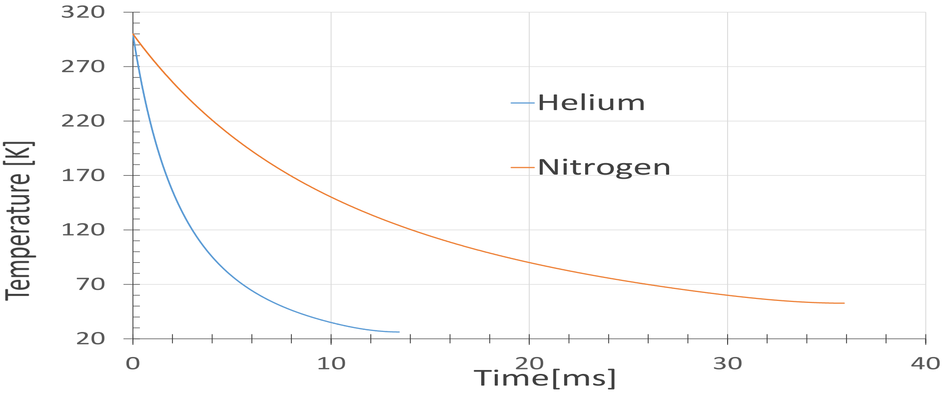

Figure 11. Comparison of Gas Temperature Evaluation Between Helium and Nitrogen.

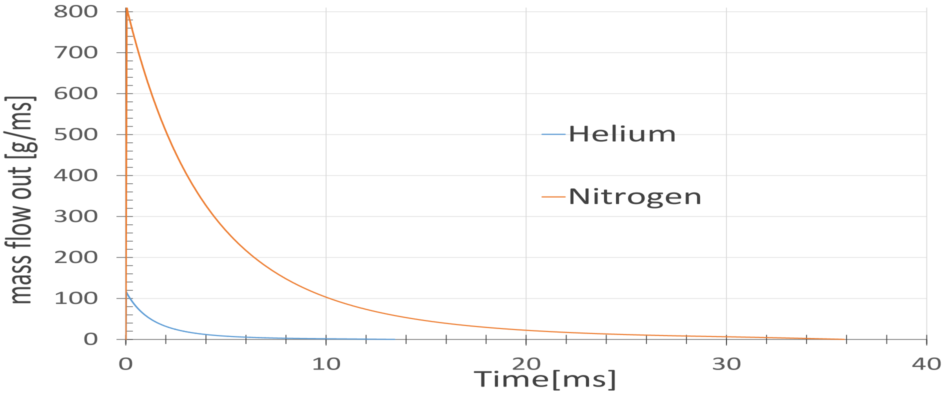

Figure 12. Comparison of Gas Mass Flow Out Evaluation Between Helium and Nitrogen.

4 Results and discussion.

4.1 Depressurization rate.

As shown in Figure 10 the depressurization rate of helium is higher than the depressurization rate of nitrogen as the vessel pressure decreases from 440 bar to 1.01325bar after 13.4292 ms in the case of using helium and after 35.88 ms in the case of using nitrogen(for the same initial conditions). This indicates that the operational period of nitrogen is about 2.5 times greater than that of helium.

4.2 Temperature decrease.

During discharging, gas temperature decreases due to gas expansion. And the gas temperatures may go beyond the design temperature range and affect the mechanical behavior of the system and the tank materials so its essential to understand the thermodynamic behavior of the stored gas during servicing for optimum design of the system. As shown in Figure 11 the temperature at the end of the discharging process is 53 k for nitrogen and 26 k for helium. so this difference in temperature must be taken into consideration when changing the operating gas from helium to nitrogen.

4.3 Mass flow rate out during the discharging process.

It is very important to Know the mass flow rate out of the vessel to the pneumatic system. And since the pressure within the vessel decreases during operation the mass flow rate out of the vessel to the system changes continuously. Figure 12illustrates the comparison between the outlet mass flow rate of helium and nitrogen. The figure shows that the outlet mass flow rate of helium is less than that of nitrogen.

5 CONCLUSIONS.

- Numerical simulation was presented and verified with an analytical solution of discharging helium and nitrogen from a cylindrical vessel.
- Numerical simulation was conducted using a Pressure-based realizable k-ϵ turbulence model with Transient-state solver in ANSYS FLUENT 18.2.
- An analytical solution was made by applying the First Law of Thermodynamics to unsteady single control volume to predict the evolution of bulk pressure, density, and temperature in vessels undergoing rapid depressurization.
- Pressure decay, gas temperature, and outlet mass flow rate out are estimated and compared with CFD simulation yielding a good agreement.
- A comparison between helium and nitrogen was presented to show how changing the working fluid would affect the operation of the pneumatic system.
- It was found that the depressurization rate of nitrogen is about 2.67 times greater than that of helium.
- The final temperature in the vessel was 26 k for helium and 53 k for nitrogen.
- Further studies shall attempt the full pneumatic system.

References

[1] Winters W S, Evans G H, Rice S F and Greif R 2012 *International journal of heat and mass transfer* **55**(1-3) 8–18 ISSN 0017-9310
[2] Johnston S C and Dwyer H A 1976 ISSN 0022-1481
[3] Artingstall G 1972 *Inst. Chem. Eng. Sympos. Ser* **33** 3–6
[4] Dhaou H, Mellouli S, Askri F, Jemni A and Nasrallah S B 2007 *International Journal of Hydrogen Energy* **32** 1922–1927
[5] Dicken C J B and Merida W 2007 *Journal of Power Sources* **165**(1) 324–336 ISSN 0378-7753

[6] Dicken C J B and Mérida W 2007 *Numerical Heat Transfer, Part A: Applications* **53**(7) 685–708 ISSN 1040-7782

[7] Suryan A, Kim H D and Setoguchi T 2012 *International Journal of Hydrogen Energy* **37**(9) 7600–7611 ISSN 0360-3199

[8] Suryan A, Kim H D and Setoguchi T 2013 *International journal of hydrogen energy* **38** 9562–9569

[9] Hasalová L, Ira J, Jahoda M and Vystrčil V 2018 Cng release from pressurized vessel through pressure relief safety device: isentropic flow approach versus cfd model *Journal of Physics: Conference Series* vol 1107 (IOP Publishing) p 042014

[10] Reynolds W C and Kays W M 1958 *Transactions of the American Society of Mechanical Engineers* **80**(5) 1160–1168 ISSN 0097-6822

[11] Melideo D, Baraldi D, Acosta-Iborra B, Cebolla R O and Moretto P 2017 *international journal of hydrogen energy* **42**(11) 7304–7313 ISSN 0360-3199

[12] Clark G L 1983 Zero-dimensional model of compressible gas flow in networks of pressure vessels: program tric

[13] Charton S, Blet V and Corriou J P 1996 *Chemical engineering science* **51**(2) 295–308 ISSN 0009-2509

[14] Woodfield P L, Monde M and Mitsutake Y 2007 *Journal of Thermal Science and Technology* **2**(2) 180–191 ISSN 1880-5566

[15] Ouellette P and Hill P 2000 *J. Fluids Eng.* **122** 743–752

[16] Magi Venkatraman Iyer J A V 2001 *Numerical Heat Transfer: Part A: Applications* **40** 317–334

[17] Melideo D, Baraldi D, Acosta-Iborra B, Cebolla R O and Moretto P 2017 *international journal of hydrogen energy* **42** 7304–7313