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CFD VALIDATION OF THE THERMODYNAMIC MODEL OF A COMPRESSED GASEOUS HYDROGEN STORAGE TANK.

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ABSTRACT

The highly abundant and friendly environmental nature of hydrogen makes it the best candidate to be considered as a replacement for current conventional energy sources, especially fossil fuel. To complete the setup of such hydrogen-based energy system, efficient hydrogen storage needs to be developed. An essential requirement toward this development is a sufficient knowledge of the dynamic behavior of the storage system. The fundamental parameters of the dynamics are thermodynamic properties, namely density, pressure and temperature. Knowing these parameters leads to developing deeper insights about the storage system in order to apply control and optimization of performance. In this research, we implemented a zero-dimensional analysis governed by ordinary differential state equations with respect to time in order to predict the important variables involved. Using this simplified thermodynamic model, we calculated the pressure and temperature of the hydrogen gas inside the storage tank based on the principles of conservation of mass and energy. Utilizing the first law of thermodynamics, we expressed the pressure and temperature as a function of time. We also developed a computational fluid dynamic (CFD) model. The equations numerically solved in the CFD model include the Navier-Stokes equation for conservation of momentum and the continuity equation for conservation of mass. We have compared the CFD model with the thermodynamic model for several initial condition assumptions to validate the results. We intend to extend this work to develop an energy storage system, including its pressure and temperature controllers.

KEY WORDS: First law of thermodynamics analysis, Compressible flow, CFD, Hydrogen Energy Storage, Fluid Dynamics, Zero-Dimensional Modeling, Heat Transfer.

1. INTRODUCTION

Hydrogen storage is one of the most difficult problems for building a hydrogen-based infrastructure. The challenge is finding the ideal storage capacity while minimizing the costs, i.e., production, operating, and maintenance, to compete with the current conventional fuel infrastructure. [2]
Most the work done so far has been dedicated to investigating temperature and pressure profiles of compressed hydrogen storage for mobile applications. Although the volume of the stationary storage is less restrictive, it takes more effort to simulate it due to its considerable size. An advantage of a simulation is that it gives us a more complete picture of the filling process with regard to developing and optimizing the storage system.

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A thermodynamic model of the storage system was developed giving pressure and temperature as a function of time. In addition, a computational fluid dynamics (CFD) model was used to validate the thermodynamic analysis. By spatial averaging of the pressure and temperature at the last time interval in the computational analysis, the final state of the system can be determined for comparison purposes. In addition, thermodynamics simulation was developed to have a complete picture of the temperature profile to compare with the CFD model. The CFD model provides parameters in many locations and time steps inside the tank to help determine a set of controllers to adjust pressure and temperature. The ultimate goal of this research is to use the thermodynamical analysis with the CFD model to determine the final state of the system.

2. FIRST LAW OF THERMODYNAMICS ANALYSIS FOR A CONTROL VOLUME

We developed a first law analysis for a control mass of hydrogen going through the filling process in a stationary tank as follows. Let the tank initially contain hydrogen gas at 1 atmosphere (*0.101 MPa*) pressure and ambient temperature 20° C. The valve is opened and the tank fills with hydrogen gas until a pressure of 50 bar (maximum capacity of the tank) is reached, and then the valve is closed. It is assumed that the tank is insulated and no heat can cross the control surface (*Q=0*). In addition, the volume is constant, hence, there is no work done (*W=0*). Figure (1) shows a schematic diagram of a control volume that includes mass transfer, the only property that can change with time in this system.

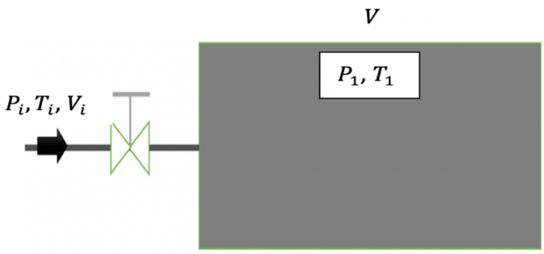

Fig. 1 Schematic diagram of the hydrogen storage tank.

Where, P stands for pressure, T for temperature, and V for volume. The ideal gas equation of state is convenient to use in thermodynamic calculations; however, it must be confirmed that conditions allow us to use it. We assumed that the incoming hydrogen temperature is known [$T_i = 200\,°C$]. Since the critical temperature for hydrogen gas is 33.2 Kelvin [1] and there is a significant difference between the critical temperature and inlet temperature, we are able to use ideal gas assumptions for evaluation of this system. Table (1) shows a summary of the known model parameters for our problem.

Table 1 Summary of the model.

Control volume	Tank
Initial state	P_1, T_1
Final state	P_2
Inlet state	P_i, T_i, V_i
Model	Ideal Gas

From the law of the conservation of mass (the continuity equation), the rate of change of mass inside the control volume can be found from the difference between the mass that comes in and the mass that goes out of the control surface. We have no flow out of the system, therefore we can write the continuity equation as

$$\Delta m = m_i \qquad (1)$$

where

$$\Delta m = m_2 - m_1 \qquad (2)$$

where m_1 is the initial mass inside the tank and m_2 is the accumulated mass.
The general form of the first law for this uniform-state, uniform-flow transient process is [1]

$$Q_{c.v.} + \Sigma m_i \left\{h_i + \frac{{V_i}^2}{2} + gZ_i\right\} = \Sigma m_e \left\{h_e + \frac{{V_e}^2}{2} + gZ_e\right\} + \left\{m_2 \left[u_2 + \frac{{V_2}^2}{2} + gZ_2\right] - m_1 \left[u_1 + \frac{{V_1}^2}{2} + gZ_1\right]\right\} + W_{c.v.} \qquad (3)$$

Where
$Q_{c.v.}$ is total heat transfer to the system.
m_e is total gas mass exits the system.
m_i is total gas mass enters the system.
$W_{c.v.}$ is total work done by the system.
h is specific enthalpy.
V is velocity.
g is acceleration of gravity.
Z is elevation.
u is specific internal energy of system.
Based on our assumptions, $Q_{c.v.} = 0$, $W_{c.v.} = 0$, and $m_e = 0$. The main objective of a most common gas rotatory-type compressor is to increase the pressure of hydrogen by putting in shaft work. The generated hydrogen enters the compressor at low pressure. As a result of shaft power input to the gas, hydrogen exits at high velocity. Then, it passes through a diffuser section where it is decelerated in a way that results in a pressure increase. Thus, hydrogen exhausts the compressor at high pressure. Also, this system is fixed in space, size, and shape. Hence, the kinetic and potential energy changes associated with the control volume are negligible. Therefore, the reduced form of the first law equation becomes

$$m_i h_i + m_i \frac{{V_i}^2}{2} = m_2 u_2 - m_1 u_1 \qquad (4)$$

Combining the continuity equation and the first law

$$\{m_2 - m_1\}\{h_i + \frac{{V_i}^2}{2}\} = m_2 u_2 - m_1 u_1 \qquad (5)$$

Simplifying and rearranging, we have

$$m_2 \left\{h_i + \frac{{V_i}^2}{2} - u_2\right\} = m_1 \left\{h_i + \frac{{V_i}^2}{2} - u_1\right\} \qquad (6)$$

We have these additional equations for the initial and final state of the mass inside the tank:

1. The ideal gas law for the mass inside the tank at the beginning of the filling process.

$$m_1 = \frac{P_1 V}{R T_1} \qquad (7)$$

where R is the hydrogen gas constant ($R = \frac{\bar{R}}{M}$, $\bar{R}$ is the gas constant and M is the molecular weight).

2. The specific volume definition for the accumulated mass at the end of the filling process.

$$m_2 = \frac{V}{v_2} \qquad (8)$$

Substituting these into the reduced form of the first law for the system we obtain

$$\frac{V}{v_2}\left\{h_i + \frac{{V_i}^2}{2} - u_2\right\} - m_1 \left\{h_i + \frac{{V_i}^2}{2} - u_1\right\} = 0 \qquad (9)$$

There are two unknowns in this equation [v_2 and u_2]. These two quantities are functions of final temperature [T_2] and final pressure [P_2]. The final pressure is the maximum pressure allowed by (or in) the tank and therefore known. Thus, there is only one value of the final temperature [T_2] for which equation

(9) will be satisfied and may be found by trial and error using the ideal gas properties of hydrogen at the different pressures. [3,6]

3. THERMODYNAMIC SIMULATION

The accumulation of mass into the system is equal to the mass which enters the system.

$$m(t + \Delta t) = m(t) + \dot{m}_i(t).\Delta t \quad (10)$$

The system contained mass m_1 at the beginning of filling the tank, so equation (10) can be written

$$m(t + \Delta t) = m_1 + \dot{m}_i(t).\Delta t \quad (11)$$

The inlet velocity and cross-sectional area of the inlet are known. Therefore, the mass at each time step can be calculated. The reduced form of the first law of thermodynamics for this case is

$$\frac{dU}{dt} = \dot{m}_i(t)\{h_i + \frac{{V_i}^2}{2}\} \quad (12)$$

The internal energy of the gas inside the storage tank is given by

$$U(t) = \mathrm{m(t)}c_v T(t) \quad (13)$$

where c_v is the amount of heat needed to increase the temperature of a control volume of *1 Kg* mass by *1 ° C* temperature [2]. From the definition of a time change and using equation (14)

$$U(t + \Delta t) = U(t) + \frac{dU}{dt}\Delta t \quad (14)$$

Thus, the internal energy at each time step can be found to be

$$U(t + \Delta t) = m(t + \Delta t)c_v T(t + \Delta t) \quad (15)$$

Consequently, we can conclude that the temperature as a function of time is

$$T(t + \Delta t) = \frac{U(t+\Delta t)}{m(t+\Delta t)c_v} \quad (16)$$

We used MATLAB to calculate the temperature throughout the process of filling the tank. The variation of the specific heat of hydrogen as a function of temperature is given in the following table [14]

Table 2 Hydrogen specific heat.

Temperature (K)	Specific Heat (kJ/kg K)
From 10K to 80K	Constant. $C_v = \frac{3}{2}R$
From 80K to 200K	Increasing from 3/2 R to 5/2 R
From 200k to 600K	Almost Constant. $C_v = \frac{5}{2}R$
From 600K to 4000K	Increasing from 5/2 R to 7/2 R

Hydrogen behaves like a monotonic gas at low temperatures; however, for increasing temperatures, its behavior is close to a diatomic gas with identical molecules.
In the current research the temperature increases from 200K to 400K, where the hydrogen specific heat was assumed to be $\frac{5}{2}R$.

4. CFD SIMULATION

The development of the CFD model has been discussed in detail in reference [2], and a summary of the conditions for the CFD model is as follows.
The simplified geometry of the stationary storage was chosen to reduce the number of mesh nodes to lower the mesh density. This helps to decrease the computer simulation time without loss of quality. The built-in material library of hydrogen properties provides all inputs required to solve the Navier-Stokes equations.
Our model combines the Laminar Flow and Heat Transfer in Fluids modules. The Heat Transfer Interface solves the Navier-Stokes equations together with an energy balance. Heat Transfer Interfaces can also solve the fully compressible form of the Navier-Stokes equations. In addition, the Laminar Flow Interface was used to compute the velocity and pressure fields for the flow of a single-phase fluid in the laminar flow regime. Another node that was implemented was the Inlet, in which a velocity field condition was used. The flow direction was assumed to be uniform through the injection pipe in the direction of the cylinder axis.
Under most practical conditions, the flow in the circular pipe is laminar for Re≪2300. By assuming laminar flow in the current research, the kinematic viscosity of the hydrogen at the temperature of the model is constant due to the density and dynamic viscosity. Therefore, the only parameters that could vary are velocity and diameter. The inlet velocity was fixed to be 10 (m/s), and instead of using a pressure boundary at the inlet for the CFD model, we have used the inflow velocity. It is not realistic to consider a constant velocity during the filling process because as the pressure inside the tank builds up, the flow velocity goes down. However, since we have a stationary tank which is very large and the simulation time is longer than the allowed computer time, we have used a constant filling velocity over the simulation time. Using a constant velocity enables us to calculate the mass flow rate. For simplicity, we have assumed that the fluid is flowing through the injection pipe at a uniform velocity. The mass flow rate is

$$\dot{m} = V_i A/\nu \qquad (17)$$

where
$\dot{m}$ is the mass flow rate, $\frac{dm}{dt}$.
V_i is the inlet velocity.
A is the cross sectional area.
ν is the specific volume.
Note that the flow is normal to the cross-sectional surface. Using the final state of the tank where the pressure is known and the temperature is found with the analysis given above, the final accumulated mass can be determined. The total time that is needed for the filling process can be obtained by using the expression of the mass flow rate along with the accumulated mass into the system

$$\Delta m = \int_0^t \dot{m}\ dt \qquad (18)$$

Substituting equation (17) into equation (18).

$$\Delta m = \int_0^t \frac{V_i A}{\nu}\ dt \qquad (19)$$

Since V_i, A, and ν are constants here,

$$\Delta m = \frac{V_i A}{\nu} \int_0^t 1\ dt \qquad (20)$$

Hence,

$$T = \frac{\nu}{V_i A} \Delta m \qquad (21)$$

Our time-dependent model has time ranging from zero to *692* seconds with a time step of *1 s* to compare with our CFD analysis results, along with the thermodynamics simulation.

A physics-controlled mesh was implemented in order to reduce numerical diffusion to a minimum.

5. RESULTS AND DISCUSSION

After the simulation was completed in COMSOL, the spatial results of pressure and temperature were exported at the corresponding times, then used to calculate the average pressure and temperature at that second using MATLAB.
The first case study is at the beginning of the filling process. The tank contains hydrogen gas at *1* atm (*0.101 MPa*) and ambient temperature of $20\,°C$. That means the tank initially possesses *3.755* kilograms of hydrogen gas ($m_1 = 3.755\ kg$).
For the next case study, the tank is half full. The half-full tank pressures and temperatures from the thermodynamic and CFD analyses are shown in Table (3). We have used the ideal gas properties of hydrogen from reference [3], and National Institute of Standard and Technology [NIST] data to calculate the temperature using equation (9).

Table 3 Pressure and temperature results for the half-full tank for two methods.

Result	Final Pressure (MPa)	Final Temperature (K)
Thermodynamics analysis	2.5	395
CFD analysis	2.0128	421.9921

The final case study was the time that the maximum pressure inside the tank is obtained. The pressures and temperatures for this case are shown in Table (4) for comparison.

Table 4 Pressure and temperature results for the full tank for two methods.

Result	Final Pressure (MPa)	Final Temperature (K)
Thermodynamics analysis	5	428
CFD analysis	5.2793	440.6655

Since the final pressure in the CFD model is higher than in the thermodynamic model, it is expected that the CFD model would have a higher final temperature. These two models support each other within good approximation limits. However, as mentioned before, a constant velocity input was used throughout the filling process in the CFD model [to reduce the simulation time] which may be the source of this inconsistency.
In figure (2), three stars show three temperatures as a function of time that were derived from the thermodynamic analysis. Also, the magenta line illustrates the temperature change during the filling for the spatial average of the storage tank exported from COMSOL. It is clear that there is a temperature jump near the beginning time due to the incoming heated hydrogen gas. After this critical time interval, the temperature increases smoothly. From the view point of storage design, this rise of temperature in an initial short time period should be considered for optimizing the costs of production.
The temperature variation during the filling shown in green line in figure (2) is calculated with MATLAB based on the thermodynamics simulation. It can be seen that the temperature is growing logarithmically. It should be noted that this calculation is based on the ideal-gas law.
For comparison of three methods, since we have used the ideal-gas law for both the thermodynamic analysis and thermodynamic simulation, these two methods show relatively good agreement. Although the CFD curve indicates higher temperature during the process, the trending appears alike with respect to the other methods.

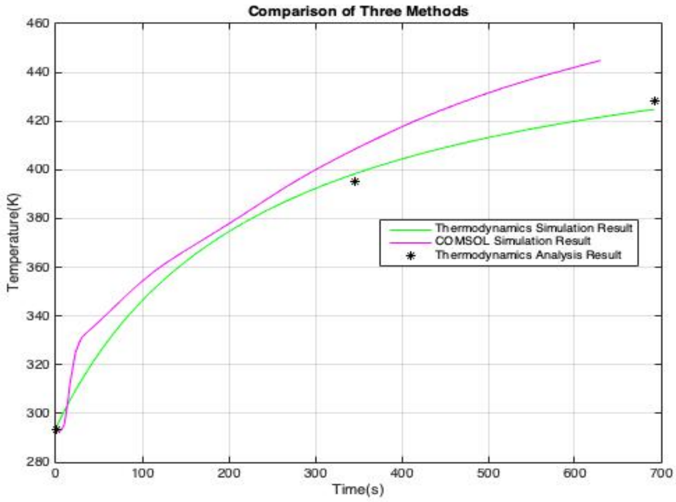

Fig. 2 Temperature as a function of time from all three methods.

Using the CFD model to scrutinize the final state of the storage tank, three cut lines have been defined to investigate the temperature profile along the tank and are shown in Fig. (3). The blue line represents the line along the center [middle of the tank where the injection pipe was located], the green line represents the line at the top of the tank, and the red line represents the line at the bottom of the tank.
It can be seen that the cutline nearest the injection pipe has the highest temperature, as expected due to the superheated gas pumped into the tank. Farther away from the input pipe, the temperatures have less variation and agree well.

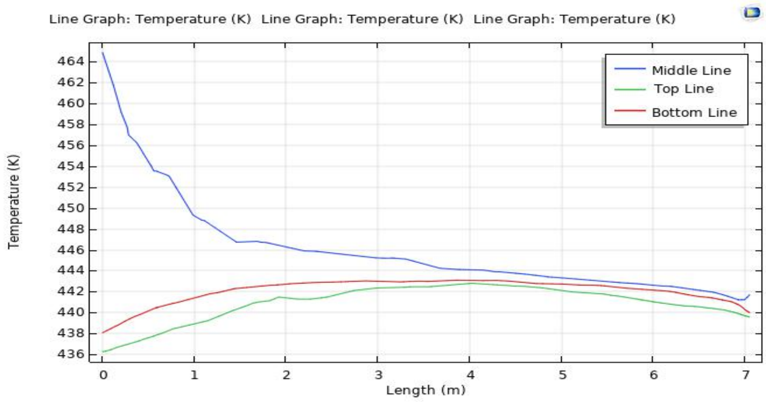

Fig. 3 Temperature at three cut-lines along the altitude of the cylinder.

Figure (4) illustrates the pressure at the same three cut-lines along the altitude of the tank.
For all 3 cut-lines, it can be seen that the pressure near the end of the injection pipe is the smallest, and it increases as we move to the opposite end of the tank.

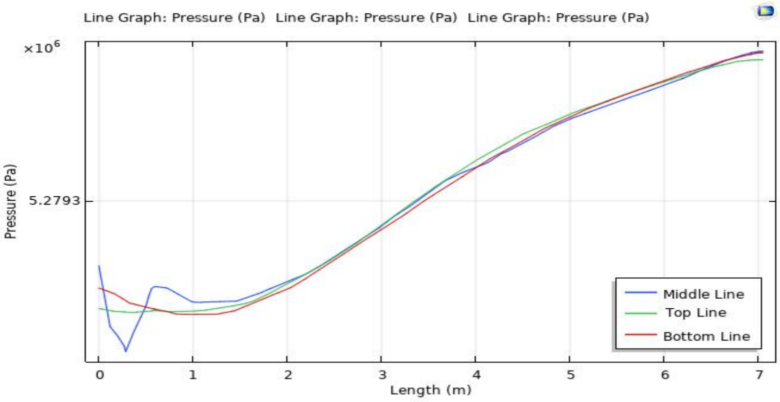

Fig. 4 Pressure at three cut-lines along the altitude of the cylinder.

Figure (5) shows the pressure development at the center of the tank. The pressure grows rapidly during the last quarter of the time period, reaching the maximum value at the end. It is useful to have such a prediction about how the pressure builds up inside the storage tank during the filling time, especially as a control aspect. It would be an important achievement to derive an empirical equation for pressure as a function of time, therefore, for designing a more precise controller.

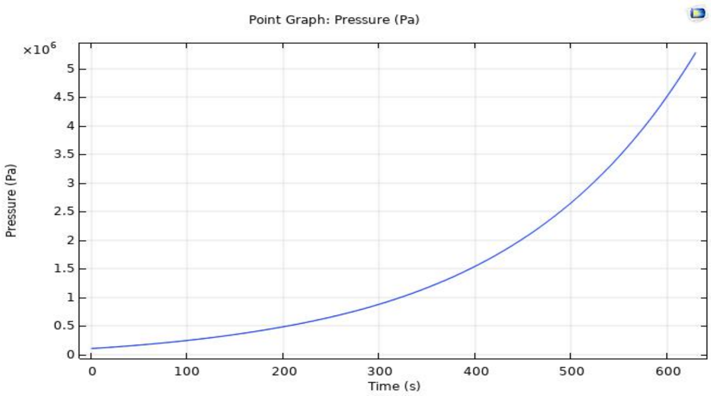

Fig. 5 Pressure vs time at the center of the tank.

6. CONCLUSIONS

Thermodynamical analyses assists in understanding the pressures and temperatures involved in filling a storage tank with hydrogen gas and provides crucial information to define simulation boundary conditions. Calculations using the CFD model have been carried out to validate a thermodynamic analysis. In addition, the CFD model gives all the useful parameters in more detail. These two models support each other within good approximation limits. It is shown that the location of the injection pipe has the highest temperature value, close to that of the incoming hydrogen. These model results could be improved by defining more precise boundary conditions, i.e., using a real gas equation instead of the ideal gas equation, and using a pressure boundary condition instead of a constant inflow velocity.

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