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Heat Analysis of Liquid piston Compressor for Hydrogen Applications

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ABSTRACT

A new hydrogen compression technology using liquid as the compression piston is investigated from heat transfer point of view. A thermodynamic model, simulating a single compression stroke, is developed to investigate the heat transfer phenomena inside the compression chamber. The model is developed based on the mass and energy balance of the hydrogen, liquid and the wall of the compression chamber at each time step and positional node with various compression ratios to calculate the temperature distribution of the system. The amount of heat extracted from hydrogen, directly at the interface and through the walls, is investigated and compared with the adiabatic case. The amount of heat transfer towards the wall is assessed according to widely used heat transfer models available in the literature.

The results show very low sensitivity of the model to different heat transfer correlations. Deviation of hydrogen temperature from adiabatic case is very small, due to large wall resistance and small contact area at the interface. Moreover, the results illustrates that the increasing of the total heat transfer coefficient at the interface and the wall will play a key role in reducing the hydrogen temperature.

Keywords: Liquid piston, Hydrogen compression, Thermodynamic model, Energy balance, Heat analysis

1. Introduction

On board High-pressure hydrogen storage is an interesting option for most of car manufacturers to provide hydrogen-powered vehicles that could compete with gasoline vehicles. This technology requires compressing and storing hydrogen above 900 bars at fueling station which increases the delivered cost of hydrogen significantly. Compression of hydrogen to such high pressures and later on cooling hydrogen down to –40°C before refueling is an area that provides strong prospects of efficiency improvement and power consumption reduction.

Nowadays, hydrogen compression is mainly performed by reciprocating compressors which encountered with several difficulties like 1) requiring a complicated compressor with many moving parts, which will be expensive to manufacture, difficult to maintain, and short-lived, 2) there is no possibility for internal-cooling during the compression processes due to the movement of solid piston, and consequently consuming a lot of energy for pre-cooling of hydrogen prior to refueling.

Novel ideas are required to improve the system functionality and make it more feasible from energy and cost point of view. Liquid piston compressor is a unique approach that can be applied to explore such prospects. As indicated by its name, in this approach the solid piston used in conventional reciprocating compressors will be replaced by liquid one. The main objective of this study is to investigate the heat transfer phenomena inside the compression chamber of this type of compressor and

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point out the critical parameters that could maximize the amount of heat which can be extracted from the compressed gas.

1.1 System configuration

The basic concept of the liquid piston compressor technology is to directly compress the gas in a compression chamber, by a column of liquid piston, driven as a part of hydraulic system. Figure 1 shows a simple P&I diagram for such system. A DC motor is coupled with hydraulic pump to generate movement of liquid flow inside the compressor chamber. During the compression stroke, the liquid will transfer the energy of hydraulic system to the pneumatic one and compress hydrogen. The hydrogen will enter the compression chamber from the inlet line, and will be released from the outlet line after it reaches to the desire pressure.

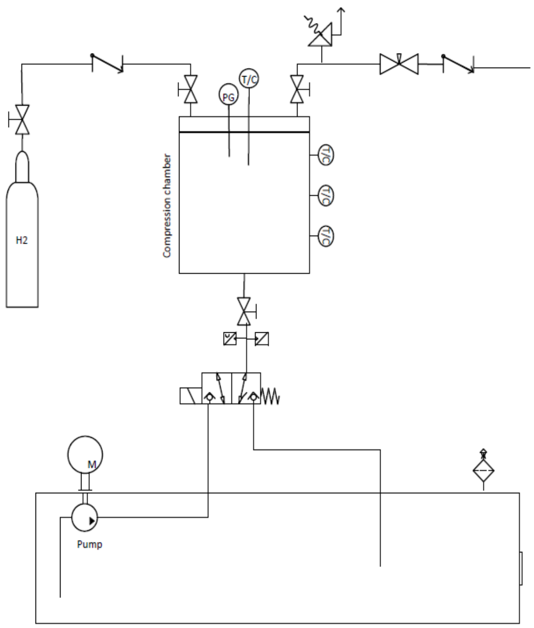

Figure 1 : simple configuration of liquid piston compressor where hydraulic pump generate liquid piston movement inside chamber using a switching valve.

The process of compressing the working gas in a liquid piston compressor in the real conditions is accompanied by a set of interrelated phenomena. Considering such interrelated processes like changes in volume, pressure and temperature of the working fluids; the influence of interface in transferring heat from gas to liquid; heat transfer of the working fluid with the structural elements, and finally the presence of thermal boundary layer close to the cylinder's wall, will add more complexity to the nature of the problem.

2. Methodology

A single compression stroke of a reciprocating liquid piston gas compression is simulated to predict the heat transfer to the liquid and wall, the system pressure, temperature and work required.

Figure 2 represents the cross-sectional view of a compression chamber and outlines its components and schematic heat transfer mechanisms between those. As it is illustrated in Figure 2, the averaged properties of liquid and gas will be estimated at each time step while the wall is discretized into n positional node. A node system can be defined with "i" as the subscript identifying a node where the heat transfer occurs. At each time step the number of nodes in contact with liquid and gas will be determined; consequently the wall temperature at each positional node will be estimated. The model is build based on the properties of hydrogen, considering it as a real gas, and water. All the properties of liquid and gas are calculated at each time step based on the estimated temperature and pressure.

The application for this analysis is a single stage compressor with a single cylinder to compress hydrogen for hydrogen refueling stations. The compressor will intake hydrogen at 100 bar and 20 C and compress it with a pressure ratio of 5:1 to 500bar when running at a frequency of 0.3 Hz. The compression chamber is a cylinder made of Stainless steel with the wall thickness of 22 mm. Inside diameter, and the stroke length of the piston are 0.08, and 0.2 m respectively. The total displaced piston volume is 0.9 l, considering the point that 10% of the volume is occupied by the liquid from the beginning to avoid the penetration of Hydrogen into the hydraulic system. The speed of compressor is controlled by adjusting the rotating speed of hydraulic pump.

The following section develops the equations for the thermodynamic model analyzing the heat transfer inside the compression chamber.

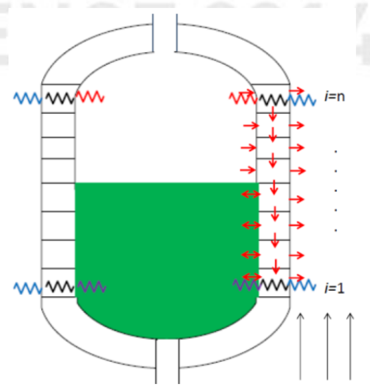

Figure 2 : the cross-sectional view of a compression chamber and schematic heat transfer mechanisms between gas, liquid and the wall.

2.1 Mass and energy balance

Since the compression will start after the inlet valve is closed, the total amount of Hydrogen trapped in the compression chamber is constant during the compression procedure. Hence, the energy conservation of the gas is determined from the first law of thermodynamics for a closed system as following:

$$\frac{dU_{gas}}{dt} = \frac{\delta Q}{\delta t} - \frac{\delta W}{\delta t} \rightarrow M_{gas}\frac{du_{gas}}{dt} = \dot{Q}_{gas} + P\frac{dV}{dt} \quad (1)$$

In eq.1, M_{gas} is the total Hydrogen mass entered the compression chamber, du_{gas}/dt is the change in internal energy of the system, $\dot{Q}_{gas}$ is the total heat rate transfer from the gas to the walls and the liquid, and PdV/dt is the rate of work which is done by the liquid on the gas side to compress hydrogen. The energy equation for the liquid has the following form

$$\frac{dU_{liq}}{dt} = \frac{\delta Q}{\delta t} - \frac{\delta W}{\delta t} - \frac{dH_{in}}{dt} \rightarrow \frac{d}{dt}(M_{liq}u_{liq}) = \dot{Q}_{liq} - P\frac{dV}{dt} + \frac{d}{dt}\sum(\dot{m}_{liq}h_{in}) \quad (2)$$

Since the liquid will be pump into the compression chamber, the dependent energy equation for open system is employed to the liquid, where dH_{in}/dt is the enthalpy flow of the liquid entering the compression chamber. The enthalpy of liquid comes into the compression chamber (h_{in}) can be estimated based on isentropic efficiency of the pump and assuming the inlet conditions of 25C and 1 atm for the liquid. Isentropic efficiency 0.7 is assumes for the pump. Moreover, $\dot{Q}_{liq}$ is the total heat rate transfer between liquid, wall and gas, and M_{liq} is the liquid mass and can be calculated for each time step based on the constant pump volume flow rate as following

$$\frac{dM_{liq}}{dt} = \sum \dot{m}_{liq} \rightarrow M_{liq} - M_{liq0} = \int_0^t \dot{m}_{liq}\, dt = \int_0^t \rho_{liq0}\, \dot{v}\, dt \quad (3)$$

Where M_{liq0} is the initial liquid mass occupied compression chamber at time t=0, $\dot{v}$ and ρ_{liq0} are the constant volume flow rate of the pump, and the inlet density of the liquid. The constant density of liquid at the inlet and outlet of the pump is assumed.

In Eq. 1 and 2, $\dot{Q}_{gas}$ and $\dot{Q}_{liq}$ can be calculated based on

$$\dot{Q}_{gas\backslash liq} = \sum_{i=m}^{i=n} \pm\dot{Q}_{W,i} \pm \dot{Q}_{interface} \quad (4)$$

Where for estimation of Q_{liq}, m=1 and n corresponds to the last node where the liquid is in direct contact with the wall. However, for the gas m is equal to the node where gas is in direct contact with the liquid and n corresponds to the total number of discretization.

2.3 Heat transfer analysis

The gas temperature will increase during the compression procedure. Due to direct contact between the gas and liquid, the heat will directly transfer from the gas to the liquid based on newton's law of cooling

$$\dot{Q}_{interface} = UA_{interface}(T_{liq} - T_{gas}) \quad (5)$$

Where $UA_{interface}$the total is heat transfer coefficient and can calculated based on conduction between liquid and gas as

$$UA_{interface} = \frac{1}{\sum R_{total}} \quad (5)$$

Where

$$\sum R_{total} = \frac{L_{liq}}{K_{liq}A} + \frac{L_{gas}}{K_{gas}A} \quad (6)$$

In eq. 5, $L_{liq\backslash gas}$ and $K_{liq\backslash gas}$ are the axial thickness and thermal conductivity of the hydrogen and water at each time step, and A is the cross sectional area of the compressor.

Moreover, due to temperature difference between hydrogen and wall of compressor, heat begins to flow into the vessel's wall through convection in which part of it will be absorbed by the liquid and the rest will be transferred to the surrounding. Liquid will behave similarly, however absorbing heat from the wall or transferring heat towards the wall by the liquid, depends on different parameter like heat transfer coefficient of the gas side, wall resistance and the total amount of external cooling. The amount of heat transfer from the liquid or gas through the wall can be calculated as

$$\dot{Q}_{W,i} = UA_{W,i}(T_{w,i} - T_{gas\backslash liq}) \quad (7)$$

In eq. 7, $T_{w,i}$ is the wall temperature at node i, and $UA_{W,i}$ is the total heat transfer coefficient which can be calculated based on total resistance of gas\liquid side and wall as

$$UA_{W,i} = \frac{1}{\sum R_{totalw,i}} \quad (8)$$

Where

$$\sum R_{totalw,i} = \frac{1}{h_i(\pi D L_i)} + \frac{\ln\left(\frac{\frac{D}{2} + \frac{t_w}{2}}{\frac{D}{2}}\right)}{2\pi L_i K_w} \quad (9)$$

Where $L_i = L/n$ and L is equal to the total length of the piston, t_w is the wall thickness, n is the total number of nodes, K_w and h_i is the thermal conductivity of the wall and heat transfer coefficient between gas\liquid and wall respectively.

The following energy balance in the wall is used to estimate the wall temperature, and the amount of heat which will transfer from the gas side towards the liquid at each positional node and time step.

$$-\dot{Q}_{w,i+1} + \dot{Q}_{axial,i+1} - \dot{Q}_{axial,i} + \dot{Q}_{sur,i+1} = 0 \quad i = 2,..,n-1 \qquad (10)$$

Where $\dot{Q}_{axial,i}$ and $\dot{Q}_{sur,i}$ stands for the axial conduction heat rate and radial convection heat rate transfer inside the wall and towards the surrounding respectively, and can be calculated as following

$$\dot{Q}_{axial,i} = K_w A_w (T_{w,i+1} - T_{w,i})/L_i \qquad (11)$$

$$\dot{Q}_{sur,i} = UA_{air}\left(T_{amb} - T_{w,i}\right) \qquad (12)$$

In eq. 9 and 10 A_w is the cross sectional area of the wall, T_{amb} and UA_{air} are the ambient temperature and the total heat transfer coefficient between outlet flow and the wall. UA_{air} in eq. 10 can be calculated based on eq.11

$$UA_{W,i} = \frac{1}{\sum R_{t,i}} \qquad (13)$$

Where

$$\sum R_{t,i} = \frac{1}{h_{sur}\pi(D+2t_w)L_i} + \frac{\ln\left(\frac{\frac{D}{2}+t_w}{\frac{D}{2}+\frac{t_w}{2}}\right)}{2\pi L_i K_w} \qquad (14)$$

Where h_{sur} in eq.14 is convection heat transfer coefficient between outlet flow and wall. In real conditions, depends on whether the wall surface is cooling naturally or by using an external cooling, h_{sur} can vary in the order of 1 to 1000 of magnitudes. In this work it is assumed that the wall will be cooled down by an external air flow with constant convection heat transfer coefficient equal to 100 W/M^2K.

Calculating the proper convection coefficient h between the compressed gas and the walls of compression chamber is the most complex part of the modeling. This is mostly due to complicated nature of the flow in short ad closed cylinders, thermal gradient across the gas, and the changing volume and surface area of the chamber.

The first step in estimation of the heat transfer coefficient for both liquid and gas side is to determine the flow regime, defined by the Reynolds number. Since a constant volume flow rate is assumed for the pump, the velocity of the liquid column is calculated based on the constant rate of piston travel as following

$$Re = \frac{\rho V D}{\mu} \quad where \quad V = \frac{\dot{v}}{A} \qquad (15)$$

It is assumed that the gas has the same velocity as the liquid all over the piston. This could be a good estimation for predicting the bulk motion of the gas, however in reality this motion will decay throughout the end of stroke. It is very desirable to keep the compression time as short as possible, therefore the flow regime inside the compression chamber is mainly turbulent which make the calculation of convection coefficient even more complicated. A fair amount of work have been done on estimation of the convection coefficient between the gas and wall of compression chamber, however due to a lot of restrictions in both experimental and numerical works none of these work are completely successful. Table 1 listed the imperial coefficients and powers obtained in widely used heat transfer correlations available in the literature. All the equations flow the general from of eq. 16.

$$Nu = ARe^a pr^b \frac{\mu}{\mu_0}^c \qquad h = \frac{Nuk}{D} \qquad (16)$$

Where in eq.16 pr, μ, k are respectively prandtl number, conductivity, viscosity of the fluid, and finally μ_0, D viscosity of the fluid at the inlet condition and the tube diameter.

Table 1: imperial coefficients and powers for seven widely used heat transfer correlations

Name	Date	A	a	b	c
Dittus-Boelter [1]	1930	0.026	0.8	0.3	0
Sieder [1]	1936	0.027	0.8	0.3	0.14
Annand [2]	1963	0.7	0.7	0.7	0
Adair [3]	1972	0.053	0.8	0.6	0
Hamilton [4]	1974	0.0245	0.8	0.6	0
Liu [5]	1984	0.75	0.8	0.6	0
Hsieh [6]	1996	0.163	1.093	0	0.15

The first correlation in Table 1 is Dittus-Boelter equation which estimated the turbulent heat transfer inside the circular tubes. Sieder suggested very similar relation to Dittus-Boelter relation; just correct it for the case of a large variation in the viscosity of the fluid. Hamilton also made used of Dittus-Boelter with slightly change.

However, in general, using Dittus-Boelter correlation is only valid for fully developed flow where L/D>60 [1]. Since, this condition does not satisfy in most of the conventional compressor chambers, especially as the stroke moves toward the top dead center position, researchers like Annand, Adair, Liu and Hsieh to use the general form of Dittus-Boelter while correcting the coefficients and powers by adopting eq. 16 with experimental data.

Annand proposed the correlation for internal combustion engines, whereas neglecting the combustion terms; the correlation could be used for the compressor.

Adair, Liu and Hsieh derived the correlation based on the experimental result obtained originally for reciprocating compressors. Though, the correlation derived by Adair were not in good agreement with instantaneous data, the averaged heat flux prediction was quite good.

In order to find the best fit for the experimental data Adair and Liu used the equation for the Reynolds number, shown in eq. 17, based on time varying equivalent diameter and swirl velocity rather than the averaged piston speed

$$Re^{*} = \frac{\rho v_s D_e}{\mu} \qquad (17)$$

And

$$De = \frac{6\ volume}{Area} = \frac{6\pi \frac{D}{2} s(t)}{\pi D s(t) + 2\pi \frac{D^2}{2}} \qquad (18)$$

Where in eq. 17, v_s is the frequency, and $s(t)$ is the piston stroke.

Shipinski [7], estimated the swirl velocity to be twice the angular velocity of the crankshaft. Since in this work, the liquid enters into the compression chamber with a constant volume flow rate, the swirl velocity, presents in eq. 19, is estimated to be twice as the frequency of compression.

$$v_s = \frac{D_e}{2} w_g \qquad (19)$$

It should be mention that for calculating the convective coefficient of liquid he general from of Dittus-Boelter equation shown in Table 1 is used. Furthermore in case of longer compression period that the gas regime will change to laminar condition general from of Dittus-Boelter equation with respect to A= 0.664, a= 0.5, b=0.3 is used.

After defining all parameters, eq. 1- 3 can be solved at the same time by using forward differencing numerical integration and updating the properties of the system at every time step based on the predicted temperature and pressure.

3. Results and discussion

The results obtained for heat analysis of reciprocating liquid piston compressor is presented in this section. The sensitivity of the model in prediction of hydrogen temperature is investigated according to different correlation shown in Table 1. Figure 3 shows the instantaneous Nu number derived from different correlations as a function of Re number. The results show a big difference between the different correlations. It can be observed that the estimated Nu number based on three correlations suggested by Hamilton, Dittus-Boelter, and Sider is very small. Though the Nu number is estimated by Adair, Annand, and Liu correlations are approximately 3, 13, times 30 larger compare to the one derived by Hamilton correlation. Moreover, it can be observed from Figure 3 that the correlation suggested by Hsieh estimated the largest Nu number which is about 67 to 80 times larger than Hamilton. Figure 3 also illustrates that the Re number which is estimated based on swirl velocity in Adair and Liu correlations, vary in smaller range compare to other correlations. As shown in Figure 3, both Re number and consequently Nu numbers based on Adair and Liu correlations have increasing trend up to 3150 whereas afterward they start to decrease. This trend can be explained by decreasing the swirl movement of the gas as the piston moves towards the top-ended center position.

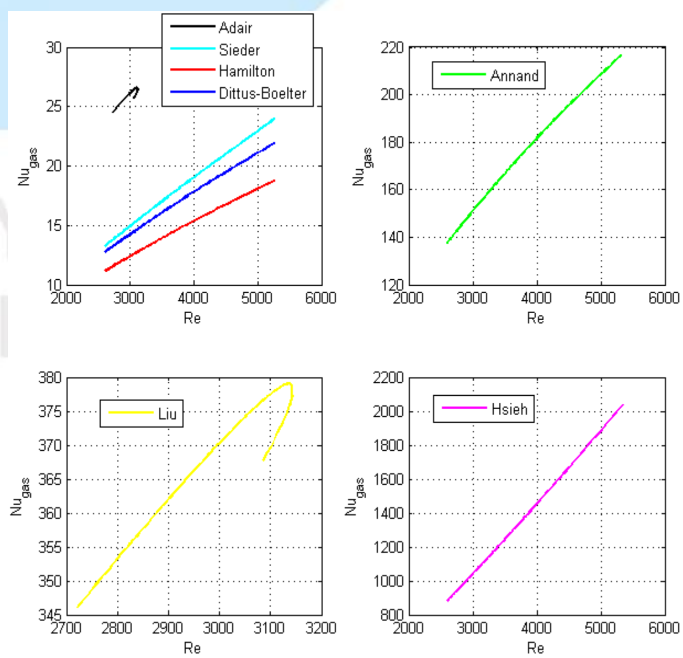

Figure 3 : Nusselt number as a function of Reynolds, calculated based on seven different correlations

As the hydrogen compressed form 100 to 500 bar, the hydrogen temperature will rise significantly. When the hydrogen temperature exceeds the temperature of the cylinder wall, all the previously described correlations will predict heat transfer into the wall. Figure 4 shows the hydrogen temperature during the compression procedure, calculated according to the seven mentioned heat transfer correlations, as well as adiabatic case, for one set of operating conditions. The results show slight deviation of Hamilton, Ditues-Boelter and sider from adiabatic case. Since these correlations estimated very small convective gas heat transfer coefficient, the amount of heat transfer toward the wall is very small. Consequently, the hydrogen temperature estimated by these correlations is very close to hydrogen temperature obtained in adiabatic case. However, lager deviations of hydrogen temperature form adiabatic condition is obtained based on other correlations.

Todescat et al. [8] compared results obtained from Annand, Adair, and Liu correlations with the numerical results of the complete Navier-Stokes equations performed by Recktenwald [9]. The comparison showed that Adair and Liu's correlations underestimate and overestimate the heat flux respectively. Nonetheless, Annand's correlation presented the best fit compering to numerical results. Moreover, in 1994, Fagotti et al. compared the results obtained from heat transfer models where Annand, Adair, Hamilton and Liu correlation used with the experimental results, and concluded that Annand model showed the best fit. It was also pointed out in this study that correlation suggested by Hamilton results in almost no heat transfer, similar to the trend observed in this study.

As it is expected, the largest deviation form adiabatic case is obtained based on Hsieh correlation in which estimated a heat transfer coefficient of the gas about 67-80 times larger than Hamilton model. However, even in this best case scenario, only 2% reduction in hydrogen is observed at 500 bar. Therefore, it can be concluded that the sensitivity of the model to different correlations is quiet low. The main reason of that can be the large resistance of the wall which practically will avoid the linear increasing of the total heat transfer coefficient with convective heat transfer coefficient of the gas.

In many prior works which have used first law of thermodynamic and heat transfer correlations for prediction of gas temperature inside the compressor wall temperature equal to ambient temperature is assumed. Such models did not take into account the wall resistance and the heat conduction through wall of the chamber, which is essential for estimation of gas temperature inside compressor.

Additionally, it can be observed from Figure 4 that the interface does not play an important role in cooling the hydrogen temperature. It should take into consideration that this model only considers the conduction mechanism between liquid and gas, but in real conditions this behavior is more complicated than this assumption which may affect the result. Therefore, validating the obtained result with an experiment is required.

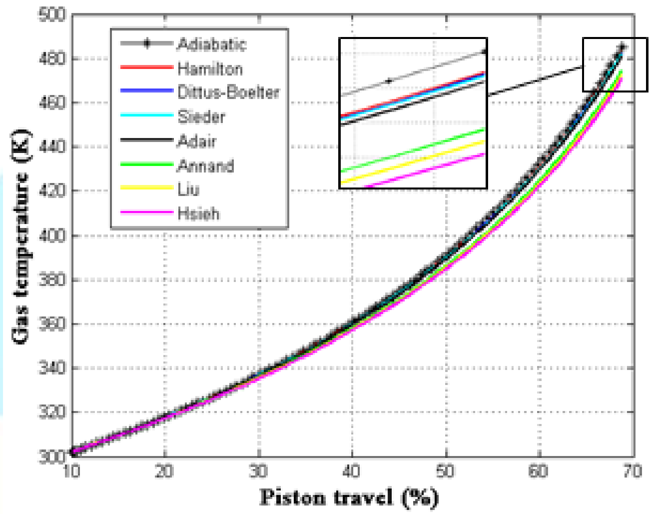

Figure 4 : Hydrogen temperature as a function of piston travel, calculated for seven different heat transfer correlations, as well as adiabatic condition.

Figure 5 shows the temperature distribution along the wall of compressor at the end of compression processes. As it is expected, the wall temperature at the top side of the compression chamber will be closer to the temperature of compressed hydrogen based on the correlations which estimated larger convective heat transfer coefficient of the gas. Nonetheless, for correlations like Adair, Sieder, Dittus-Boelter and Hamilton the temperature obtained at the top side of the vessel will deviate about 27%, 27%, 28%, and 30% form the hydrogen temperature respectively, at 19 cm from bottom of the vessel. The red and blue color in Figure 5 represents the space inside the compression chamber occupied by hydrogen or water at the end of compression processes respectively. Wall temperature distribution shows that for the nodes which are in direct contact with hydrogen the temperature is above 340 K, whereas it decreases considerably as going towards the bottom side of the compressor chamber. The bottom side of the compression chamber has almost the same temperature as water all the time during compression.

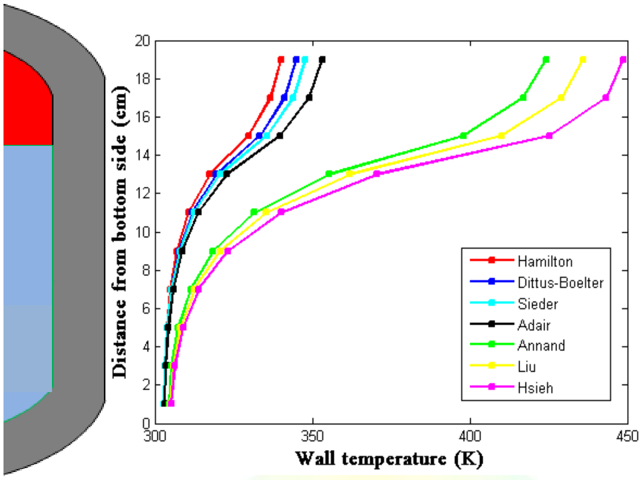

Figure 5: Temperature distribution in cylinder wall

Eq. 5, 7, and 12 show that increasing the total heat transfer coefficient both at interface and the wall will increase the amount of heat flux and consequently reduction of hydrogen temperature. Figure 6 andFigure 7 show the changes of temperature and pressure during 3 seconds and 22 seconds of compression, assuming the total heat transfer coefficient in 2000 times larger than it is estimated based on eq. 6.

The results show 8-9% and 25% temperature reduction during the compression compare to adiabatic case, at 500 bar corresponds to 69% of piston travelling. Since in this case the reduction of temperature is mainly due to considerable heat flux at the interface, the two heat transfer correlations behave similarly and the two curves are matched very well for longer compression processes.

Figure 7 shows lower pressure compare to adiabatic cases for the mentioned scenarios. The main reason of such behavior can be explained by significant reduction of temperature due to considerable increase of heat flux at interface.

Increasing the total heat transfer coefficient up to 2000 times more than what is estimated requires increasing the area up to the same amount. This is practically not passible by increasing the diameter versus the length of cylinder. Spraying the liquid into compression chamber could increase the contact area between liquid and gas considerably, but still requires a detailed modeling to estimate the total amount of heat that could be removed based on such technology.

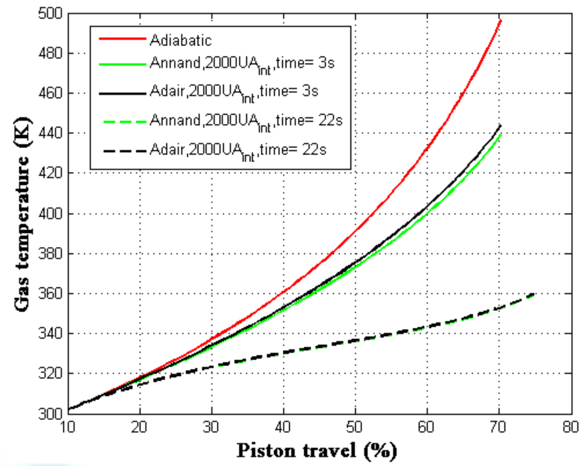

Figure 6 : Hydrogen temperature as a function of piston travel, changing critical parameters related to heat transfer at the interface

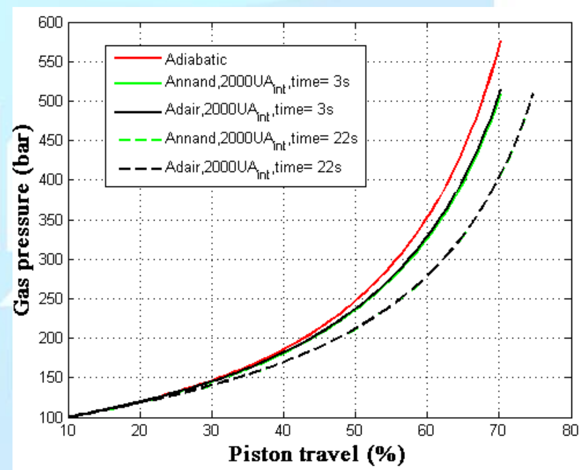

Figure 7 : Hydrogen pressure as a function of piston travel, changing critical parameters related to heat transfer at the interface

Furthermore increasing the total heat transfer coefficient between gas and wall, liquid and wall, and air and could also play role in decreasing the hydrogen temperature. Figure 8 shows, if the total heat transfer coefficient in both eq. 7 and 12 increase up to 100 times more than what is estimated in this model, the hydrogen temperature will decrease up to 23% and 29% according to Adair and Annand correlations compare to adiabatic case, at 500 bar corresponds to 69% of piston travelling. Increasing the total heat transfer coefficient up to 100 times larger than what is estimated is required a considerable increasing of the geometry from inside and outside of the compressor which practically is very difficult to reach. Compare to previous case, for this case time could not play an important role in the results. Since longer compression time will decrease the speed of hydrogen and water considerably, therefore the flow regime will change to laminar condition and will not follow the correlations mentioned in Table 1 anymore. The heat transfer coefficients of the hydrogen and liquid will decrease in laminar regime, hence decreasing the total heat transfer coefficient.

Hydrogen Pressure, Figure 8, during the compression will behave similarly as shown in for previous case, mainly due to the significant reduction of temperature.

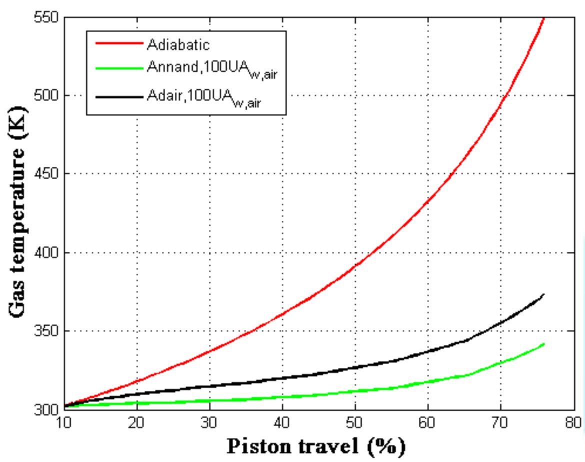

Figure 8 : Hydrogen temperature as a function of piston travel, changing critical parameters related to convective heat transfer towards the wall

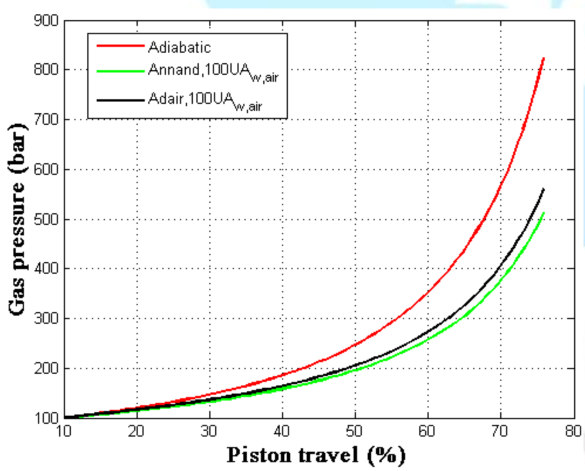

Figure 9 : Hydrogen pressure as a function of piston travel, changing critical parameters related to convective heat transfer towards the wall.

4. Conclusion

This work presents a study on heat transfer analysis of liquid piston compressor. The model is build based on the first law of thermodynamics in case of reciprocating liquid compressor to predict the system' s temperature and pressure at different time steps The amount of heat transferred form the hydrogen towards the interface and the wall is estimated according to widely used heat transfer models, available in the literature. The results show small changes in hydrogen temperature compare to adiabatic case, due to large wall resistance and small contact area between gas and liquid at the interface. Furthermore, Sensitivity analysis of the model based on total heat transfer coefficient both for the interface and the wall proves the key role of this parameter in reduction of hydrogen temperature during the compression procedure.

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