PARAMETRIC STUDY OF HYDROGEN FILLING PROCESS IN TYPE IV TANK BASED ON CFD SIMULATION

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Abstract. Currently, with the gradual increase in the use of automobiles, the use of fossil fuels is also gradually increasing, which inevitably brings about the problem of environmental pollution. Fuel cell vehicles use hydrogen as an energy source, and high-pressure hydrogen storage is widely used to store the hydrogen needed for fuel cell vehicles. The safe and efficient storage of hydrogen is a technical difficulty that restricts the development of fuel cell vehicles. This paper takes the real gas equation of state and thermodynamic conservation equation as the theoretical basis, and uses COMSOL Multiphysics to carry out a modelling study on the hydrogen filling process. It was indicated that the mass flow rate has a large effect on both the pressure and the temperature of the hydrogen in the tank and a reasonable setting of the mass flow rate can reduce the pressure and temperature for a certain filling mass. In addition, the final temperature and pressure of hydrogen decreases as the inlet temperature decreases, and pre-cooling is an effective way to reduce the temperature of the hydrogen tank. The final temperature and pressure of the hydrogen in the tank decreases as the filling time increases. The higher the initial pressure of hydrogen, the shorter the time required for filling and the lower the final temperature of hydrogen. Meanwhile, the final SOC (State of Charge) of hydrogen becomes larger as the initial pressure increases. The results of the study are of guiding significance for the optimal design of hydrogen filling strategies in hydrogen refuelling stations.

Keywords: hydrogen, filling, hydrogen storage tank, CFD simulation.

Introduction

As a renewable carrier, hydrogen energy shows potential as an ideal alternative energy source for the world of the future. At present, many scholars have carried out research on the problems related to hydrogen filling. Miguel et al. [1] have experimentally investigated Type III and Type IV hydrogen storage tanks rated at 70 MPa, respectively. Li et al. [2] developed a two-dimensional axisymmetric CFD model to study the temperature variation of hydrogen storage tank during rapid hydrogen filling. De et al. [3] researched the influence of different initial temperatures on the thermal effects of the hydrogen storage tank filling process. A CFD model of the filling process was established to simulate the filling process under different initial temperature conditions. It was shown that the higher the initial temperature, the higher the final hydrogen temperature. Galassi et al. [4] used ANSYS as a platform to establish a three-dimensional CFD model of a Type IV 29L hydrogen storage tank, and used experimental data as a comparison to prove the correctness of the predicted results of the CFD model. Li et al. [5] studied the rapid hydrogen filling process of hydrogen adding tank through experiments and CFD simulation. Several key parameters in the rapid filling process were studied. Therefore, it is crucial to design a rational fast filling strategy. Galassi [6] further investigated the CFD modelling accuracy which turbulence was adopted as the flow model and Redliche-Kwong was used as the model’s base conservation equation to simulate the filling process of the Type IV hydrogen tank, and the accuracy of the CFD model was proved by comparing it with a number of sets of experiments. Melideo et al [7] investigated the effect of pre-cooling on the final temperature of the hydrogen storage tank in case of rapid filling (filling time less than 3 minutes). Simonovski et al. [8] investigated the key parameters that have an impact on the filling temperature during rapid filling. Li et al [9] built a CFD model based on thermodynamic theory to analyse the hydrogen charging process of the hydrogen storage tank. Zheng et al. [10] studied the filling strategy of hydrogen refuelling stations. Li et al. [11] studied the influence of different geometries and different inlet channels on the hydrogen temperature. Chen et al. [12] investigated the true gas equation of state during hydrogen filling. In this study, a simplified form of the equation of state is proposed to describe the real state of hydrogen, and the accuracy of the proposed hydrogen equation of state is higher than that of existing models.

In this paper, we will take the Type IV 29L hydrogen storage tank as the study objective to investigate the influence of hydrogen filling parameters on the thermal effect of hydrogen, which will serve as a referent for the safe and rapid hydrogen filling in future hydrogen refuelling stations.

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Governing equations and model validation

The equations involved in the hydrogen filling process are as follows. Mass conservation equation:

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0, \tag{1}$$

where ρ – density of hydrogen, kg·m^{-3};
t – time, s;
u – velocity vector;
p – pressure, Pa.

Momentum conservation equation:

$$\rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla)u = \nabla \cdot \left[-pI + \mu(\nabla u + (\nabla u)^T) - \frac{2}{3}\mu(\nabla \cdot u)I\right] + F, \tag{2}$$

where μ – kinetic viscosity of hydrogen, Pa·s;
I – unit vector;
F – volumetric force vector, N·m^{-3}.

Energy conservation equation:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p u \cdot \nabla T + \nabla \cdot q = Q, \tag{3}$$

where c_p – specific heat capacity of hydrogen, J·(kg·K)$^{-1}$;
T – temperature, K;
q – heat flux vector, W·m^{-2}.

Since the pressure and temperature inside the hydrogen storage tank are very high during the hydrogen filling process, the hydrogen inside the tank will seriously deviate from the properties of the ideal gas, and the real gas equation of state must be used to describe the state of hydrogen. From the literature [12], this paper adopts the empirical equation of the real gas to describe the temperature-pressure relationship of hydrogen, which is closer to the actual state of hydrogen. The actual gas equation of state:

$$z = \frac{pv}{RT} = \left(1 + \frac{\alpha p}{T}\right), \tag{4}$$

where $\alpha = 1.9155 \times 10^{-6}$ K·Pa^{-1}.

The heat conduction equation of the tank wall:

$$\rho c \frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\lambda \frac{\partial T}{\partial z}\right) + \boldsymbol{\Phi}, \tag{5}$$

where τ – time, s;
ρ – density, kg·m^{-3};
c – specific heat capacity, J·(kg·K)$^{-1}$;
$\boldsymbol{\Phi}$ – source term.

Newton's law of cooling involved in convective heat transfer processes:

$$q = h(T_{\mathrm{w}} - T_f), \tag{6}$$

where q – heat flux, W·m^{-2};
h – heat transfer coefficient, W·(m^2·K)$^{-1}$;
T_{w} – temperature of the tank wall, K;
T_f – ambient temperature, K.

Based on the actual parameters of the hydrogen storage tanks a CFD model was built and meshed in COMSOL software. According to the spatial location of the experimental [1] thermocouples, this paper identifies three points in the model as the detection points of temperature and pressure. The coordinates of the three points are shown in Fig. 1, which indicates the relative positions of the three points and the inlet of hydrogen, and the three points are point 1 (0, 108.5), point 2 (55, 85.5), and point

3 (107, 105.5). The pressures at the three points are the same, and the pressure at any one of the points is used to represent the hydrogen pressure, and the average temperature of the three detected points is used to represent the hydrogen temperature. In the experiment, the filling time of the hydrogen storage tank was 252 s, the initial temperature was -8 °C, the initial hydrogen mass was 34.1 g, and the final hydrogen mass at the end of restart was 648.3 g.

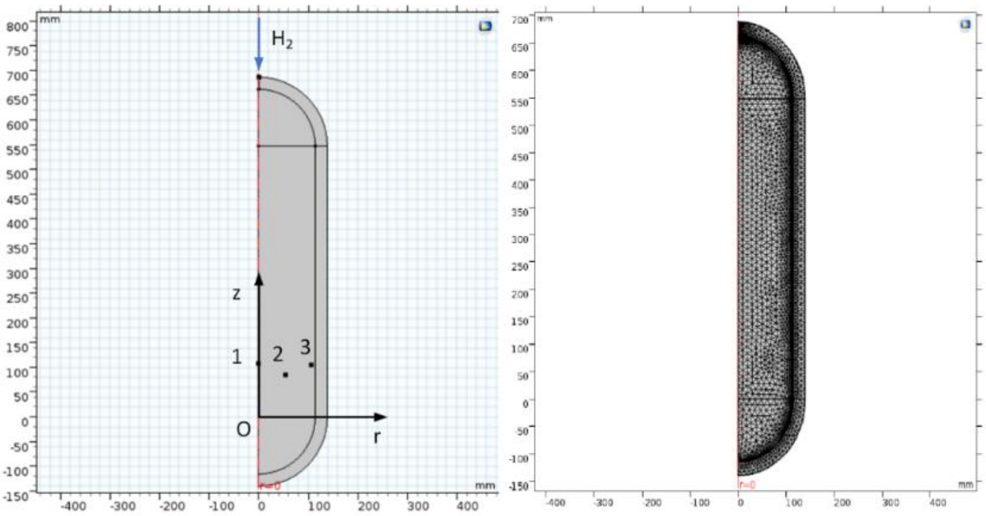

Fig. 1. **Schematic geometric model and meshing of Type IV 29L hydrogen storage tanks**

The average temperature and pressure of the experiment are compared with the simulation results as shown in Fig. 2(a) and Fig. 2(b), respectively. In the temperature comparison validation of hydrogen storage tank, the maximum error between the calculated and experimental temperatures is 8%, and the temperature reaches the highest by the final moment, in which the calculated temperature is 89 °C and the experimental temperature is 88 °C. From the comparison of this set of experimental data with the calculated temperature, it can be seen that the laminar flow model can well simulate the temperature changes in the hydrogen storage tank during hydrogen filling. On this basis, the laminar flow model was continued to be used to verify the pressure of the hydrogen storage tank, as shown in Fig. 2(b). The calculated pressure is basically the same as the experimental pressure, so the laminar flow model can better simulate the thermal effect of the hydrogen storage tank during the hydrogen filling process.

Parametric study of CFD models

In the experiment [1] of the Type IV 29L hydrogen storage tank, the initial hydrogen mass was 0.034 kg and the final mass was 1.04 kg. As shown in Fig. 3, the experimental mass flow rates and the theoretical mass flow rates are listed, and the three theoretical mass flow rates are the assumed mass rates under the condition of ensuring the same final hydrogen mass in the tank. Rate 1 is a linearly increasing flow rate from zero to a maximum rate of 8.2 g·s^{-1}, rate 2 is constant at 4.2 g·s^{-1} and rate 3 is a linearly decreasing flow rate from 8.2 g·s^{-1} to zero.

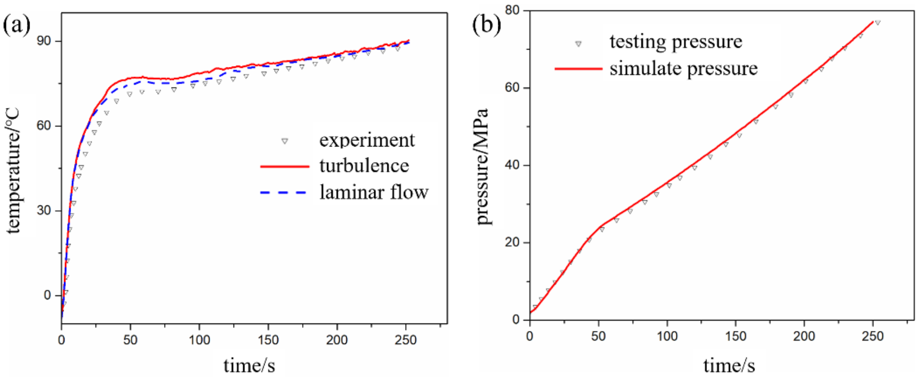

Fig. 2. **Temperature (a) and pressure (b) verification of hydrogen storage tanks**

Under the original laminar flow model, these three mass flow rates are used as the inlet conditions to obtain the pressure and temperature change curves of hydrogen in the tank with different mass flow rates and compare them with the experimental values. Fig. 3(b) and 3(c) show the pressure and temperature of hydrogen at different mass flow rates compared to the experimental data, respectively. As seen in Fig. 3(b), the final pressure does not vary much during the filling process, but the trend varies widely. From Fig.3(c), it is seen that the hydrogen temperature rises continuously for all two rates except rate three. The reason for the difference in rate three is that after the peak temperature, the mass flow rate gradually decreases, at the same time the hydrogen transfers heat outward, and the energy of the filled hydrogen is less than the energy transferred to the tank wall, resulting in a decrease in the hydrogen temperature inside the tank. From Table 1 it can be seen that the final pressure inside the tank is the lowest at 73.7 MPa for mass flow rate I and highest at 77.8 MPa for mass flow rate III. When inflated at the rate of the experiment, the maximum hydrogen temperature was the lowest at 88.1 °C and the rate one corresponded to the highest hydrogen temperature at 98.8 °C.

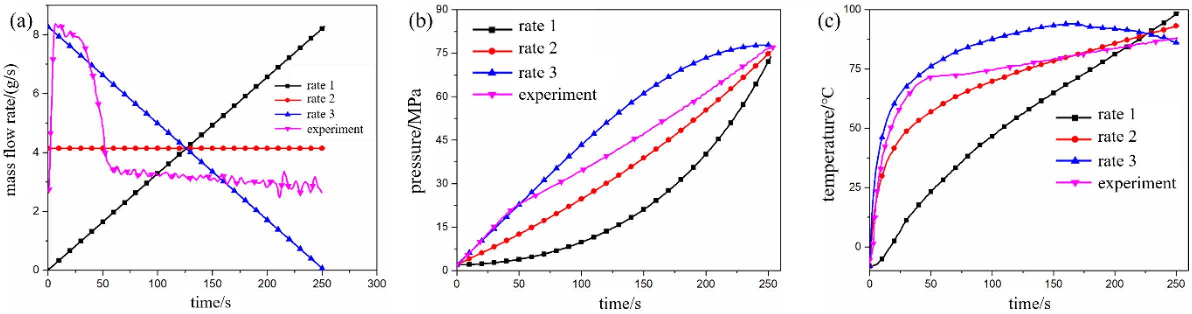

Fig. 3. **Inlet mass flow rates (a), pressure (b) and temperature (c)**

According to the data of calculation and comparison, it can be concluded that: in the case of a certain mass of filling, the filling rate is first large and gradually becomes small, the temperature of hydrogen is relatively low; the filling rate is first small and gradually becomes large, the temperature of hydrogen is relatively high. The change in rate does not have much influence on the final pressure inside the tank. Hydrogen refuelling stations need to fill the hydrogen storage tanks in a short time, which causes the hydrogen temperature to rise rapidly. A valid solution to this problem is in pre-cooling. Based on the original laminar flow model, the hydrogen filling temperature (23 °C) was reduced by 10 °C, 20 °C, 30 °C and 40 °C, respectively. Then calculation was performed to obtain the data of pressure and temperature changes in the hydrogen storage tank after pre-cooling. As it can be seen from Fig. 4(a) and Fig. 4 (b), the maximum pressure and maximum temperature of the hydrogen decreased with the gradual decrease of the inlet temperature. When the filling temperature was room temperature (23 °C), the maximum pressure and temperature of hydrogen were 77 MPa and 89.5 °C, respectively, which exceeded the safety standards of 70 MPa and 85 °C. As the temperature of the precooled hydrogen decreases, the maximum pressure and temperature of the hydrogen in the tank decreases. The final data is shown in Table 2, where the maximum temperature is lower than 85 °C at 10 °C pre-cooling, but the final pressure exceeds 70MPa; at 40 °C pre-cooling, the safety criteria for both pressure and temperature are met. This data suggests that hydrogen pre-cooling is a useful method of reducing the maximum temperature and pressure with constant filling mass.

Table 1

Final pressure, final temperature and maximum temperature for different mass flow rates

Mass flow rate	**Final pressure, MPa**	**Final temperature, °C**	**Highest temperature, °C**
Experimental values [1]	77.0	88.1	88.1
Rate 1	73.7	98.8	98.8
Rate 2	75.6	93.4	94.4
Rate 3	77.8	86.0	86.0

In this section, a Type IV 29L on-board hydrogen storage tank is investigated to examine the effect of the filling time on the thermal effect of the tank while ensuring the same final mass of filling. In the experiment of 29L hydrogen storage tank [1], the initial hydrogen mass in the tank is 0.049 kg, and the final mass is 1.090 kg. Since there are different filling times, the corresponding filling rates are different for each group of models. Table 3 below shows the different filling times and the corresponding average filling rates.

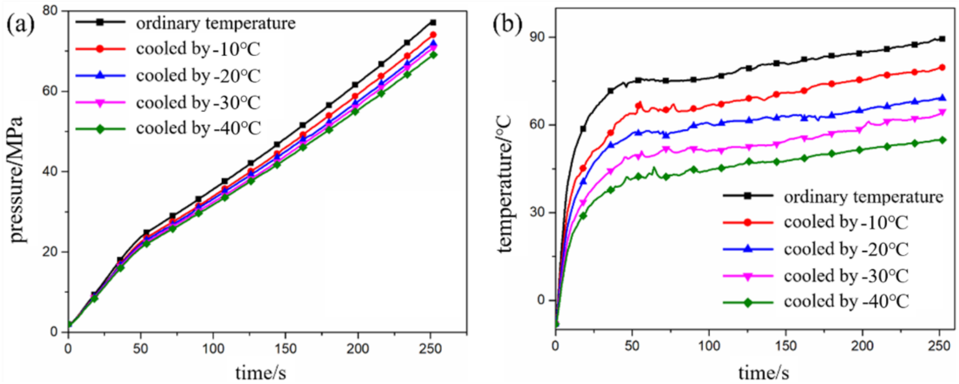

Fig. 4. **Pressure(a) and temperature(b) data at different pre-cooling temperatures**

Different filling times and filling rates are used as conditions for the laminar flow model, and calculations are carried out separately to obtain the pressure and temperature relationships corresponding to different filling times, as shown in Fig. 5(a) and Fig.5(b). As shown in Fig. 5(a), the final pressure exceeds 70 MPa in each filling time from 100 s to 700 s. When the filling time is 100 s, the filling rate is the fastest, the pressure inside the tank rises sharply during the filling process, and the final pressure is also the highest. As the filling time increases, the filling rate decreases and the final pressure inside the tank becomes smaller. The final pressure was 78.3 MPa at a filling duration of 700 s. The final pressures are 80.1 MPa and 79.4 MPa when the filling time is 500 s and 600 s. It can be seen that when the filling time is long enough, the increase of the filling time will not have a great influence on the final pressure of hydrogen. Fig. 5(b) shows that the final temperature of the hydrogen gradually decreases as the filling time increases. The final temperature of hydrogen is the highest when the filling time is 100s, which reaches 117.3 ºC. The final temperature of hydrogen is higher than 85 ºC when the filling time is from 100 to 400s. While the maximum hydrogen temperatures in the tank were 81.2 ºC and 76.9 ºC at filling times of 600 s and 700 s, respectively, which were lower than the nominal temperature of 85 ºC in the Type IV hydrogen storage tank.

Table 2

Final pressure and final temperature for different inlet temperatures

Inlet temperature	Final pressure, MPa	Final temperature, ºC
Experimental values [1]	77.0	89.5
Pre-cooling -10 ºC	74.0	79.6
Pre-cooling -20 ºC	71.9	69.2
Pre-cooling -30 ºC	70.8	64.6
Pre-cooling -40 ºC	69.1	54.9

Table 3

Different filling times and corresponding filling rates

Filling time, s	100	200	300	400	500	600	700
Average rate, g·s^{-1}	10.4	5.2	3.5	2.6	2.1	1.7	1.5

It is seen that an appropriate extension of the filling time has less influence on the final pressure inside the tank and more effect on the final temperature. Since the initial and final masses in the tank are fixed, and the pressure of hydrogen is mainly affected by the mass of hydrogen, the filling time decreases the final pressure by 10.4% from the filling time of 100s to 700s. Even if the filling time is further doubled, the final pressure of hydrogen is hardly lower than 70 MPa. In contrast, the temperature is more affected by the filling time, and the final temperature is reduced by 34.4% from the filling time of 100s to 700s. In summary, in the filling process of the tank, under the premise of guaranteeing the quality of hydrogen filling, appropriately increases the time of hydrogen filling, which can reduce the final temperature of the hydrogen significantly, making the hydrogen temperature comply with the safety standards. Appropriately extending the filling time can also reduce the final pressure of hydrogen, but the effect is not obvious, especially when the quality of hydrogen is certain, the effect of hydrogen filling time on reducing the final pressure is insignificant.

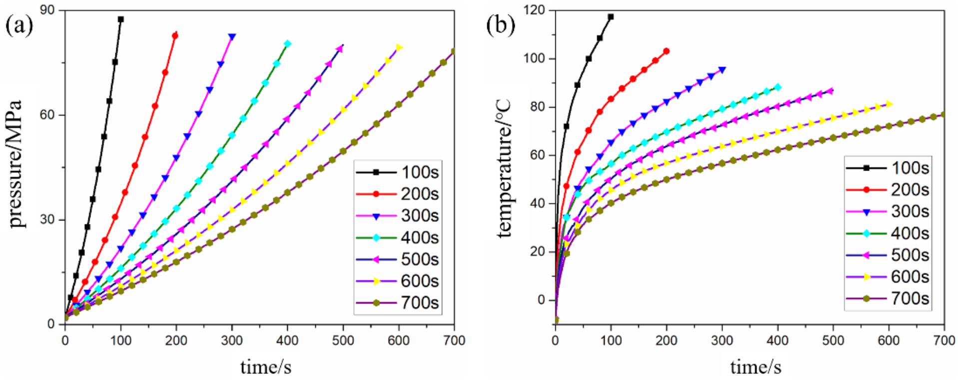

Fig. 5. **Pressure(a) and temperature(b) for different filling times**

In this section, a Type IV 29L hydrogen storage tank is used as a research object to investigate the effect of different initial pressures on the temperature. According to the actual filling conditions, the initial hydrogen temperature inside the tank is set to 23 ºC, and the filling rates are all constant at 4 g·s^{-1}. In this section, four different initial pressures are assumed to investigate the connection between the initial pressure and final temperature. The initial data are shown in Table 4. The filling time for each working condition is shown in Table 5. Based on the actual gas equation of state the filling time for each condition was calculated, and then the initial conditions are imported into the laminar flow model to obtain the curves of temperature versus time under different initial pressure conditions as shown in Fig. 6(a). As it can be seen in Fig. 6(a), at an initial pressure of 2MPa, the temperature inside the hydrogen storage tank reaches 97.8 ºC at the end of filling. When the initial pressure is 10MPa, the final hydrogen temperature reaches 89.8 ºC. Temperatures in both of these operating conditions exceeded 85 ºC. In contrast, the final hydrogen temperatures in Case III and Case IV were 78.0 ºC and 56.6 ºC, respectively, both of which are lower than the safety temperature of 85 ºC for Type IV hydrogen storage tanks.

Table 4

Initial hydrogen mass in the tank for different initial conditions

Parameter	Condition 1	Condition 2	Condition 3	Condition 4
Initial pressure, MPa	2	10	20	30
Initial hydrogen mass, g	49	224.8	421.6	597

Table 5

Filling times for different operating conditions

Parameter	Condition 1	Condition 2	Condition 3	Condition 4
Initial pressure, MPa	2	10	20	30
Filling time, s	231	191	148	110

It can be seen that the lower the initial pressure of hydrogen, the longer the filling time, making the final temperature of hydrogen higher. If the initial pressure can be increased appropriately, the maximum pressure of 70MPa can be met, while meeting the safe temperature of 85 ºC in the tank. However, according to the actual conditions of use of the vehicle, the higher the initial pressure, the lower the mass of hydrogen to be filled, so the initial pressure should not be too high. Planning the hydrogen filling time according to different hydrogen filling rates and initial pressures of different hydrogen storage tanks at the hydrogen refuelling stations can be a guideline for the hydrogen filling strategy at the hydrogen refuelling station. In the filling protocol issued by the American Society of Automotive Engineers, SOC of a hydrogen storage tank during filling is a very important reference indicator. SOC is the ratio of the density of the hydrogen storage tank in the actual state to the density in the standard case.

$$\mathrm{SOC} = \frac{\rho(p,T)}{\rho(70\mathrm{MPa},15^{\circ}\mathrm{C})} \times 100\% \, . \tag{7}$$

The SOC values for the four operating conditions are shown in Fig. 6(b). As shown in Fig. 6(b), at a final filling pressure of 70 MPa, SOC increases as the initial filling pressure increases, and the larger the SOC, the larger the mass of hydrogen in tank. The reason for this is that the higher the initial pressure, the lower the final temperature, resulting in more hydrogen in the tank.

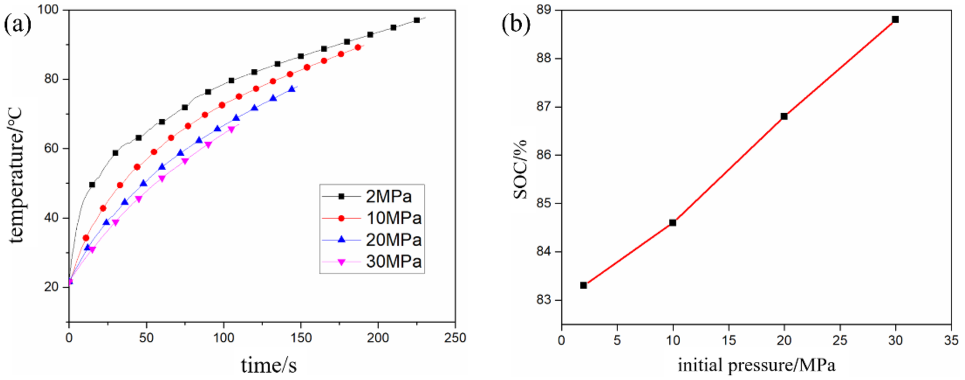

Fig. 6. **Filling temperatures(a) and SOC(b) in four working conditions**

Conclusions

In this study, a CFD model of the two-dimensional axisymmetric hydrogen filling process is established using the finite element simulation software COMSOL as a platform. The influence of the filling rate, filling temperature, filling time and the initial pressure on the thermal effect of hydrogen are investigated separately. It can be a guide for safe and efficient filling of hydrogen.

1. The mass flow rate has a large effect on both the pressure and the temperature of the hydrogen in the tank. The final pressure and temperature in the tank are lower when the hydrogen inlet is from fast to slow, and the final pressure and temperature in the tank are higher when the hydrogen inlet is from slow to fast. Changing the mass flow rate can reduce the pressure and temperature.
2. Changing different inlet temperatures reveals that when the inlet temperature is lowered, the final temperature and pressure of the hydrogen are lowered. This indicates that pre-cooling is an effective method to reduce the temperature of the tank.
3. In the study of the effect of different filling times on the hydrogen temperature, when the filling time increases, the final pressure of filling decreases, but the percentage decrease is small. As the filling time increases, the temperature also decreases, by a larger percentage.
4. Appropriately increasing the initial pressure for filling can reduce the final temperature of hydrogen and increase the total final hydrogen mass in the tank.

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