A DUAL ZONE THERMODYNAMIC MODEL FOR REFUELING HYDROGEN VEHICLES

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ABSTRACT

With the simple structure and refueling process, the compressed hydrogen storage system is currently widely used. However, thermal effects during charging-discharging cycle may induce temperature change in storage tank, which has significant impact on the performance of hydrogen storage and the safety of hydrogen storage tank. In our previous works, the final hydrogen temperature, the hydrogen pre-cooling temperature and the final hydrogen mass during refueling process were expressed based on the analytical solutions of a single zone (hydrogen gas) lumped parameter thermodynamic model of high pressure compressed hydrogen storage systems. To address this issue, we once propose a single zone lumped parameter model to obtain the analytical solution of hydrogen temperature, and use the analytical solution to estimate the hydrogen temperature, but the effect of the tank wall is ignored. For better description of the heat transfer characteristics of the tank wall, a dual zone (hydrogen gas and tank wall) lumped parameter model will be considered for widely representation of the reference (experimental or simulated) data. Now, we extend the single zone model to the dual zone model which uses two different temperatures for gas zone and wall zone. The dual zone model contains two coupled differential equations. To solve them and obtain the solution, we use the method of decoupling the coupled differential equations and coupling the solutions of the decoupled differential equations. The steps of the method include: (1) Decoupling of coupled differential equations; (2) Solving decoupled differential equations; (3) Coupling of solutions of differential equations; (4) Solving coupled algebraic equations. Herein, three cases are taken into consideration: constant inflow/outflow temperature, variable inflow/outflow temperature and constant inflow temperature and variable outflow temperature. The corresponding approximate analytical solutions of hydrogen temperature and wall temperature can be obtained. With hydrogen temperature and hydrogen mass, the hydrogen pressure can be calculated with using the equation of state for ideal gas. Besides, the two coupled differential equations can also be solved numerically and the simulated solution can also be obtained. The SAE J2601 developed a standard fueling protocol based on the so-called MC Method to a formula based approach, as an extension of the early look-up table approach. This study will help to set up another formula based approach of refueling protocol for gaseous hydrogen vehicles.

Keywords: hydrogen storage; refueling; fast filling; thermodynamics; heat transfer; safety

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Nomenclature

a_{in}	heat transfer coefficient of inner surface, W/m^2/K	T	temperature of hydrogen, K
a_{out}	heat transfer coefficient of outer surface, W/m^2/K	T_0	initial temperature in tank, K
A_{in}	inner surface area of tank, m^2	T_f	temperature of ambient *fluid*, K
A_{out}	outer surface area of tank, m^2	T_w	temperature of tank wall, K
c_p	constant-pressure specific heat, kJ/kg/K	T_{w0}	initial temperature of tank wall, K
c_v	constant-volume specific heat, kJ/kg/K	T_∞	hydrogen inflow temperature, K
c_w	Specific heat of tank wall, kJ/kg/K	T^*	under constant inflow/outflow temperature, $T^* = \gamma' T_\infty + \alpha' T_f$, K
h	specific enthalpy of hydrogen, J/kg		under variable inflow/outflow temperature, $T^* = \alpha' T_w$, K
h_{in}	specific enthalpy of inflow hydrogen, J/kg	u	specific internal energy, J/kg
h_{out}	specific enthalpy of outflow hydrogen, J/kg	V	volume of tank, m^3
m	hydrogen mass in tank, kg	Z	compressibility factor
$\dot{m}$	hydrogen mass flow rate, kg/s	***Greek symbols***	
m_0	initial hydrogen mass in tank, kg	α	dimensionless heat transfer coefficient, $\alpha = a_{\mathrm{in}} A_{\mathrm{in}} / (c_v \dot{m})$
$\dot{m}_{\mathrm{in}}$	hydrogen mass inflow rate, kg/s	α'	under constant inflow/outflow temperature, $\alpha' = \alpha/(1+\alpha)$
$\dot{m}_{\mathrm{out}}$	hydrogen mass outflow rate, kg/s		under variable inflow/outflow temperature, $\alpha' = \alpha/(1+\alpha-\gamma)$
m_w	mass of tank wall, kg	γ	ratio of specific heats, $\gamma = c_p/c_v$
p	hydrogen pressure, MPa	γ'	$\gamma' = \gamma/(1+\alpha)$
R	universal gas constant, $R = 8.314$J/K/mol	μ	fraction of initial mass, $\mu = m_0/m$
t	time variable, s	μ'	$\mu' = \mu^{1+\alpha}$
t^*	characteristic time, $t^* = m_0/\dot{m}$, s	τ	dimensionless time, $\tau = t/t^*$
t_w^*	$t_w^* = m_w c_w / (a_{\mathrm{in}} A_{\mathrm{in}})$	τ_w	$\tau_w = t/t_w^*$

1 INTRODUCTION

Hydrogen is considered to be one of the most potential fuels to deal with the exhaustion of natural resource, environmental pollution and global warming, and the compressed hydrogen gas cylinder is currently widely used to store the hydrogen due to its simplicity in tank structure and refueling process. However, for safety reason, the final gas temperature in the hydrogen tank during vehicle refueling must be controlled under a certain limit, e.g., 85℃ [1-3].

To achieve this goal and ensure the safety during charge and discharge processes, many experiments have been done to find how the refueling parameters affect the hydrogen temperature and hydrogen pressure. The University of British Columbia measured the effects of different initial hydrogen mass and different filling time on the rise of hydrogen temperature for a type III tank with 74L [4]. The Kyungil University and Chung Ang University conducted experiments to research the charge cycle for a type IV tank with four different initial pressures of 5MPa, 10MPa, 15MPa and 20MPa [5]. The JRC-IET (Institute for Energy and Transport, Joint Research Centre of the European Commission) utilized the GasTeF facility to carry on the experiments for studying the thermal behavior during charging-discharging cycle of an on-board hydrogen tank [6-8]. Zheng conducted experiments to research the temperature rise and built a CFD model to measure the effects of initial pressure and ambient temperature on it [9]. In addition to the experimental research, there are also so much theoretical analysis and numerical simulations on the compressed hydrogen system. Yang presented a thermodynamic and heat transfer analysis of the refueling process of a gaseous hydrogen fuel tank [10]. The Japan automobile research institute simulated the fast filling process of a hydrogen tank [11]. The University of Ontario Institute of Technology built a lumped parameter model to measure the effects of initial hydrogen pressure and initial hydrogen temperature on the thermal behavior during fast filling process [12]. The JRC-IET also built a three-dimensional numerical model to simulate the thermal effects during fast filling for a type III tank and a type IV tank respectively [13, 14].

Recently, the SAE J2601 standard “Fueling Protocols for Light Duty Gaseous Hydrogen Surface Vehicles” [1, 2] is adopted to control final temperature of refueling and to optimize the refueling procedure. Appendix H of the SAE J2601 standard describes the MC method which has some advantages beyond the table-based method [3], such as faster and more consistent fueling times, wider range of dispenser fuel delivery temperatures. The MC method considers the heat capacity of the tank wall but it uses single temperature for both the hydrogen gas and the tank wall. i.e., the MC method is a dual zone, single temperature model, and this single temperature is higher than wall temperature but lower than the gas temperature. In our preview works, a single zone and single temperature lumped parameter model was presented [15]. We only consider the gas zone and obtain the solution of hydrogen temperature with ignoring the effect of the tank wall. Now we extend this model to dual zone and dual temperature model which includes hydrogen and tank wall. For gas zone, we combine the mass balance equation and energy balance equation to obtain a differential equation, then we solve it with the assumption the tank wall temperature is constant and we can obtain an algebraic equation. For wall zone, similarly another algebraic equation can also be obtained on the basis that the gas temperature is constant. The two algebraic equations can be coupled by a characteristic temperature. Then, we solve coupled algebraic equations and obtain the analytical solutions of hydrogen temperature and wall temperature. Besides, with the analytical solution of hydrogen temperature and the solution of mass balance equation, we also calculate the hydrogen pressure during the whole cycle. Afterwards, we use

Matlab/Simulink software to express our thermodynamic model, and the corresponding simulated solution can also be obtained. By comparing the analytical solution and the simulated solution, we can check the validity of our model, and improve our model.

2 MASS AND ENERGY EQUATIONS FOR THE DUAL ZONE MODEL

For the charging and discharging processes in a compressed hydrogen storage system, the mass and energy balance equations can be written as:

$$\frac{dm}{dt} = \dot{m}_{\text{in}} - \dot{m}_{\text{out}} \tag{1}$$

$$\frac{d(mu)}{dt} = \dot{m}_{\text{in}}h_{\text{in}} - \dot{m}_{\text{out}}h_{\text{out}} + A_{\text{in}}a_{\text{in}}(T_w - T) \tag{2}$$

$$\frac{d(m_w c_w T_w)}{dt} = A_{\text{in}}a_{\text{in}}(T - T_w) - A_{\text{out}}a_{\text{out}}\left(T_w - T_f\right) \tag{3}$$

where $\dot{m}_{\text{in}}$ and $\dot{m}_{\text{out}}$ are the inflow and outflow rates of hydrogen mass respectively, while h_{in} and h_{out} are the specific enthalpy of inflow and outflow hydrogen respectively. Herein, we define $\dot{m} = \dot{m}_{\text{in}}$ and $\dot{m}h = \dot{m}_{\text{in}}h_{\text{in}}$ for charging process, $\dot{m} = -\dot{m}_{\text{out}}$ and $\dot{m}h = -\dot{m}_{\text{out}}h_{\text{out}}$ for discharging process. We assume that the tank wall has sufficient hear capacity that there is no heat transfer from the outer surface of the tank wall to the ambient, i.e., $a_{\text{out}} = 0$. Eq.(1) to Eq.(3) become:

$$\frac{dm}{dt} = \dot{m} \tag{4}$$

$$\frac{d(mu)}{dt} = \dot{m}h + A_{\text{in}}a_{\text{in}}(T_w - T) \tag{5}$$

$$\frac{d(m_w c_w T_w)}{dt} = A_{\text{in}}a_{\text{in}}(T - T_w) \tag{6}$$

3 ANALYTICAL SOLUTION OF DUAL ZONE MODEL

3.1 Charge/discharge processes under constant inflow/outflow temperature

During the charge process, assuming $\dot{m}$ is constant, thus the solution of Eq.(4) is $m = m_0 + \dot{m}t$. So Eq.(5) becomes:

$$\dot{m}u + (m_0 + \dot{m}t)\frac{du}{dt} = \dot{m}h + A_{\text{in}}a_{\text{in}}(T_w - T) \tag{7}$$

With expressions of the specific internal energy $u = c_v T$, the specific enthalpy $h = c_p T_\infty$ and the ratio of specific heats $\gamma = c_p/c_v$, Eq.(7) becomes:

$$\frac{dT}{dt} = (1+\alpha)\frac{T^* - T}{t^* + t} \tag{8}$$

where $T^* = \gamma' T_\infty + \alpha' T_w$, $\gamma' = \gamma/(1+\alpha)$, $\alpha' = \alpha/(1+\alpha)$ $\alpha = a_{\text{in}}A_{\text{in}}/c_v/\dot{m}$, and $t^* = m_0/\dot{m}$.

Denoting $t_w^* = m_w c_w/(a_{in}A_{in})$, the energy balance equation for wall zone becomes:

$$\frac{dT_w}{dt} = \frac{T - T_w}{t_w^*} \tag{9}$$

Eq.(8) and Eq.(9) are the two coupled differential equations. To obtain the analytical solutions of hydrogen temperature and wall temperature, we need to decouple these two differential equations. Herein, we solve the Eq.(8) with the assumption that the wall temperature in Eq.(8) is constant and solve the Eq.(9) with the other assumption that hydrogen temperature in Eq.(9) is also constant.

Solution of gas temperature under assumption of constant wall temperature

Denoting $\tau = t/t^*$, with the initial condition $T = T_0$ at $t = 0$, the solution of Eq.(8) is obtained:

$$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1+\tau}\right)^{1+\alpha} \tag{10}$$

This is the analytical solution of hydrogen temperature. As to the solution of mass balance equation $m = m_0 + \dot{m}t$, it can be rewritten as $m/m_0 = 1 + \dot{m}t/m_0$, $m/m_0 = 1 + t/t^*$ or $\mu = 1/(1+\tau)$. Thus, the solution of hydrogen temperature can be written in the form of "rule of mixture":

$$T = f_g T_0 + \left(1 - f_g\right) T^* \tag{11}$$

where $f_g = \mu' = \mu^{1+\alpha} = \left(\frac{1}{1+\tau}\right)^{1+\alpha}$, is the weighted factor, $\mu = m_0/m$ is the initial mass ratio.

Solution of wall temperature under assumption of constant gas temperature

With the initial condition $T_w = T_{w_0}$ at $t = 0$, we obtain the solution of Eq.(9):

$$\frac{T - T_w}{T - T_{w_0}} = e^{-\tau_w} \tag{12}$$

Eq.(12) is the solution of wall temperature. here $\tau_w = t/t_w^*$. Denoting $f_w = e^{-\tau_w}$, the solution of wall temperature can also be written in the form of "rule of mixture":

$$T_w = f_w T_{w_0} + (1 - f_w) T \tag{13}$$

Noting $T^* = \gamma' T_\infty + \alpha' T_w$ makes the algebraic equations Eq.(11) and Eq.(13) coupled, they can be solved simultaneously.

$$T = \frac{f_g T_0 + \gamma'\left(1 - f_g\right) T_\infty + \alpha'\left(1 - f_g\right) f_w T_{w_0}}{1 - \alpha'\left(1 - f_g\right)(1 - f_w)} \tag{14}$$

$$T_w = \frac{f_w T_{w_0} + f_g (1 - f_w) T_0 + \gamma'\left(1 - f_g\right)(1 - f_w) T_\infty}{1 - \alpha'\left(1 - f_g\right)(1 - f_w)} \tag{15}$$

The hydrogen temperature T and wall temperature T_w can be expressed by the corresponding refuelling parameters such as initial hydrogen temperature, inlet temperature, initial wall temperature and so on.

3.2 Charge/discharge processes under variable inflow/outflow temperature

For the case of variable inflow/outflow temperature, the inflow or outflow temperature is supposed to be the same with the hydrogen in tank, i.e., $T_\infty = T$. Herein, we use the same method as section 3.1, solving the energy balance equation for gas zone with the assumption the tank wall temperature is constant and solving the energy balance equation for wall zone with the other assumption the hydrogen temperature is also constant, thus equation (8) turns to be:

$$\frac{dT}{dt} = (1 + \alpha - \gamma)\frac{T^* - T}{t^* + t} \tag{16}$$

where $T^* = \alpha' T_w$, $\alpha' = \alpha/(1 + \alpha - \gamma)$. With the initial condition $T = T_0$ at $t = 0$, the solution of Eq.(16) is:

$$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1+\tau}\right)^{1+\alpha-\gamma} \tag{17}$$

This is the analytical solution of hydrogen temperature for the case of variable inflow/outflow temperature. Herein, we also define $f_g = \left(\frac{1}{1+\tau}\right)^{1+\alpha-\gamma}$, Eq.(17) can also be written in the form of “rule of mixture”, which shares the same from as Eq.(11). For this case, the analytical solution of wall temperature is not changed in the form as Eq.(13). The new characteristic temperature $T^* = \alpha' T_w$ makes them coupled, and we can calculate:

$$T = \frac{f_g T_0 + \alpha' f_w (1 - f_g) T_{w_0}}{1 - \alpha'(1 - f_g)(1 - f_w)} \tag{18}$$

$$T_w = \frac{f_w T_{w_0} + f_g (1 - f_w) T_0}{1 - \alpha'(1 - f_g)(1 - f_w)} \tag{19}$$

3.3 Dormancy process

The energy balance equations for gas zone and wall zone can be written as following:

$$\frac{d(mu)}{dt} = a_{in} A_{in} (T_w - T) \tag{20}$$

$$\frac{d(m_w c_w T_w)}{dt} = a_{in} A_{in} (T - T_w) \tag{21}$$

During dormancy process, the hydrogen mass is constant. Herein we also use $u = c_v T$, divided Eq.(21) by Eq.(20), it is obtained:

$$\frac{m c_v}{m_w c_w} \frac{dT}{dT_w} = -1 \tag{22}$$

Eq.(22) shows the function relationship between hydrogen temperature and wall temperature. We define $k = m_w c_w / (m c_v)$, with the initial condition $T = T_0$, $T_w = T_{w_0}$, we can obtain solution of Eq.(22):

$$T = T_0 + k\left(T_{w_0} - T_w\right) \tag{23}$$

Combining this solution with the energy balance equation for wall zone, we obtain:

$$\frac{dT_w}{dt} = A T_w + B \tag{24}$$

where $A = -(k + 1)/t_w^*$ and $B = \left(T_0 + k T_{w_0}\right)/t_w^*$. With initial condition $T_w = T_{w_0}$ at $t = 0$, the solution of Eq.(24) can be obtained:

$$T_w = \left(T_{w_0} + \frac{B}{A}\right) e^{At} - \frac{B}{A} \tag{25}$$

Substituting this equation into Eq.(23)

$$T = T_0 + k\left[T_{w_0} - \left(T_{w_0} + \frac{B}{A}\right)e^{At} + \frac{B}{A}\right] \quad (26)$$

3.4 Pressure during charge-discharge cycle

During charge-discharge cycle, the hydrogen pressure in the tank will change as time goes by. Due to the safety requirement, the maximum working pressure is not allowed to exceed 125% of the nominal working pressure, so it is necessary for us to monitor the hydrogen pressure. We can use the equation of state for ideal gas to calculate the hydrogen pressure as following:

$$p = \frac{mRT}{VM_{H_2}} \quad (27)$$

In this article, we have obtained the expressions of hydrogen temperature T and hydrogen mass m from above sections. And the hydrogen pressure can be calculated by giving a certain volume of a tank. Besides, the equation of state for real gas such as $p = Z\frac{mRT}{VM_{H_2}}$ and the Redlich-Kwong equation can also be used to obtain the hydrogen pressure, they will be considered further.

4 RESULTS AND DISCUSSION

The thermodynamic equations and solutions for the processes in charge-discharge cycle are summarized in Table.1 and the values of the parameters used for solving the thermodynamic equations are listed in Table.2. With these values, not only the analytical solutions can be obtained, but also the simulated solutions can be obtained with using Matlab/Simulink software as shown in Fig.1. Herein, three cases simulated solutions are presented, case 1, constant inflow/outflow temperature; case 2, variable inflow/outflow temperature; case 3, constant inflow temperature and variable outflow temperature. Fig.2(a) shows the variation of the hydrogen temperature with time. The hydrogen temperature is increasing during charge process as hydrogen gas flows in with energy, and decreasing during discharge process because of the hydrogen gas being delivered from inside tank to outside tank, during the two dormancy cycles, the hydrogen temperature changes due to the heat exchange being existing between the hydrogen gas and the wall tank. Fig.2(b) shows the variation of the wall temperature with time. Fig.2(c) shows the variation of the hydrogen pressure with time.

During the three cases mentioned above, the case 3 (constant inflow temperature and variable outflow temperature) is supposed to be close to the reality. we use our model and thermodynamic equations to obtain the analytical solutions. The comparisons between the analytical solutions and the simulated solutions are shown in Fig.3. Fig.3(a) shows the variation of the hydrogen temperature with time, Fig.3(b) shows the variation of the wall temperature with time, Fig.3(c) shows the variation of the hydrogen pressure and the hydrogen mass (the dot dash line) with time. The deviations between the analytical solution and the simulated solution may be caused by the assumptions when we solve the coupled differential equation.

For the case 3, according to the simulated solution, the minimum and maximum wall temperatures are respectively 300K and 314K. In our model, we can fix the wall temperature as 300K and 314K, when the wall temperature is fixed, the dual zone model is simplified to be the single zone model, the solutions of the hydrogen temperature under these two cases can be set as the lower bound and upper bound. The deviations between the bound situations and the solutions of hydrogen temperature are shown in Fig.4. It can be found that the analytical solution and the simulated solution are somewhere between the two bound situations.

5 CONCLUSION

The thermodynamic behaviors for charging-discharging cycle of compressed hydrogen system can be described by a dual zone thermodynamic model. According to the model, the energy equations for the gas zone and the wall zone are two coupled differential equations, the solutions for the gas zone and the wall zone are two coupled algebraic equations. With the corresponding assumptions, the approximate analytical solutions of hydrogen temperature and wall temperature can be obtained. With the analytical solution of hydrogen temperature and the solution of mass balance equation, the variation of hydrogen pressure on time can be calculated with using the equation of state for ideal gas if a certain volume of a tank is given. The simulated solutions are also obtained by using Maltab/Simulink, which can be used to compare with the analytical solutions and to improve our model.

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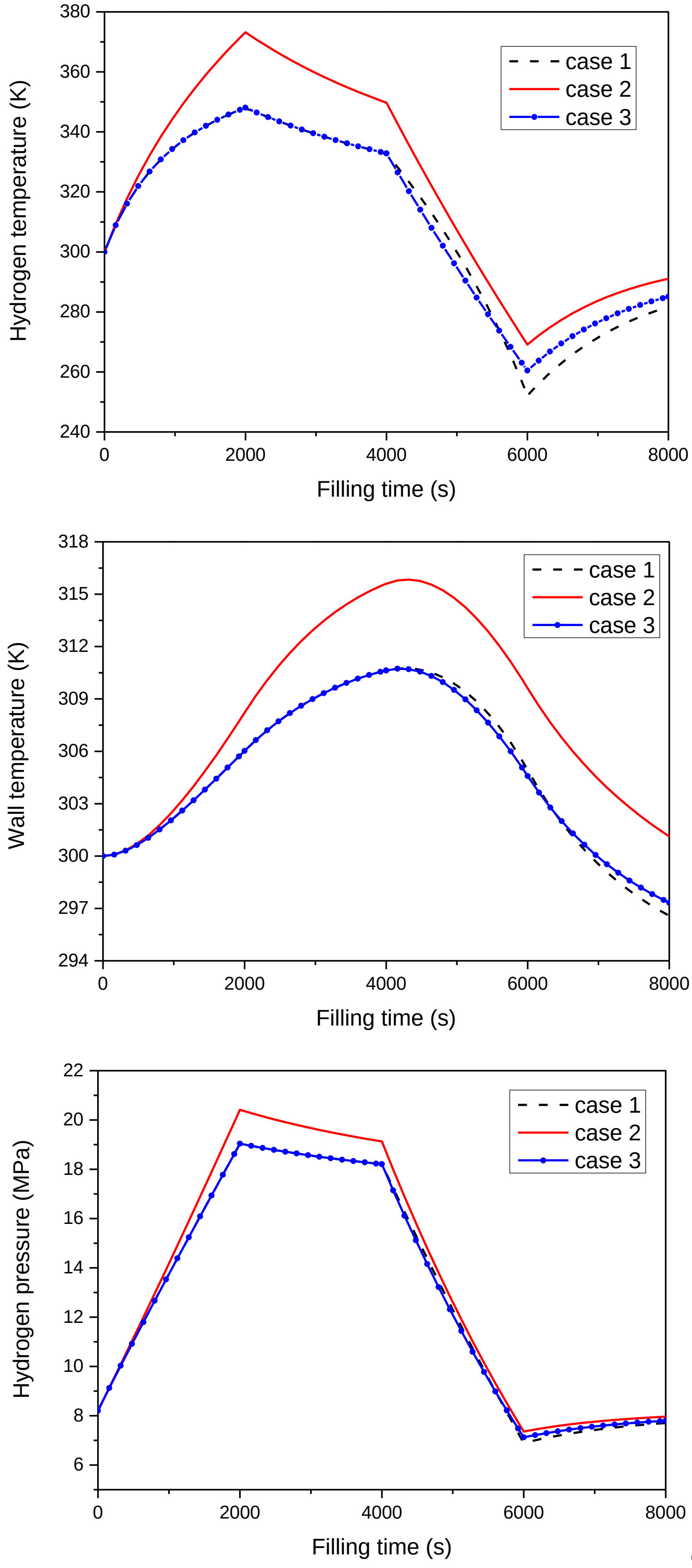

a)

b)

c)

Figure.2 Simulated solutions for the three cases (case 1, constant inflow/outflow temperatures; case 2, variable inflow/outflow temperatures; case 3, constant inflow temperature and variable outflow temperature).

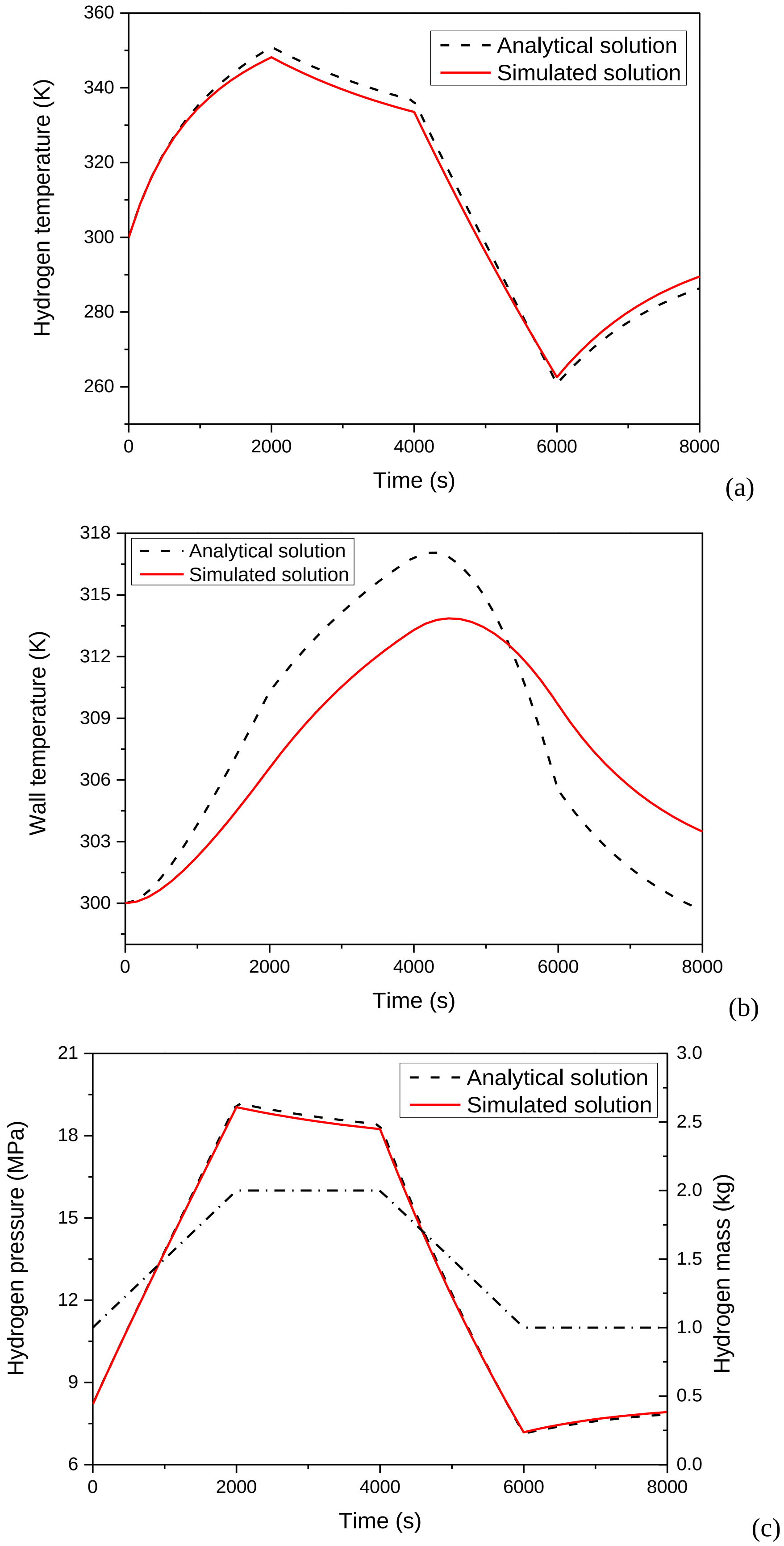

Figure.3 Analytical and simulated solutions for case 3 (constant inflow temperature and variable outflow temperatures)

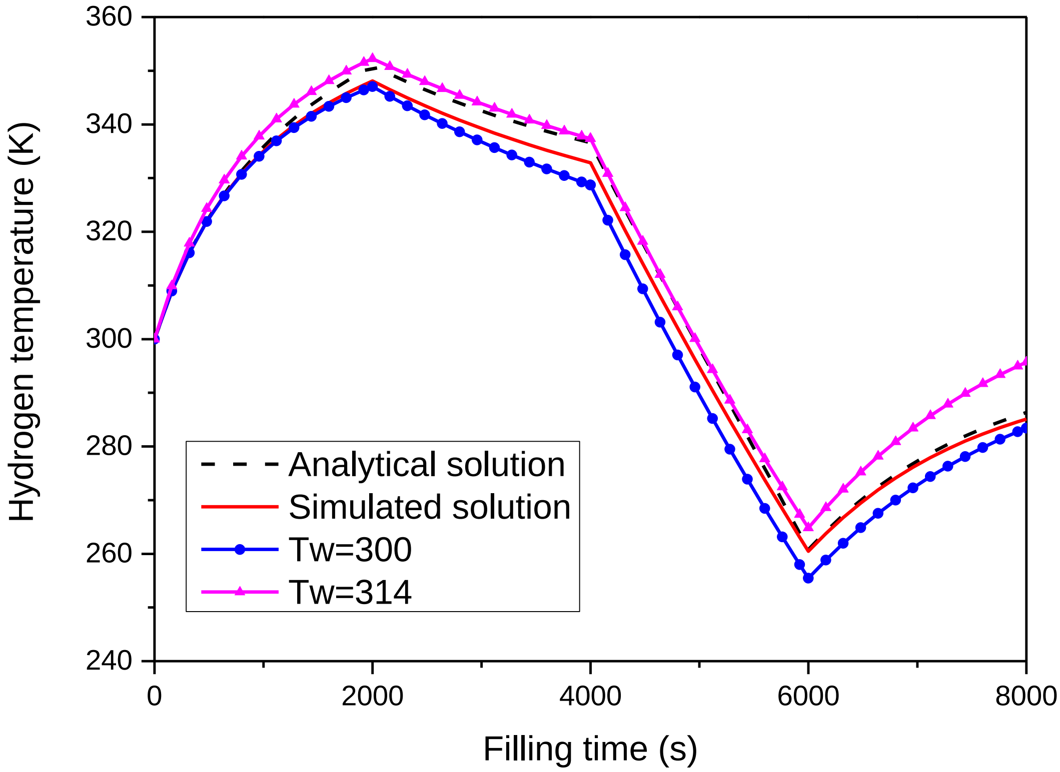

Figure.4 The comparison between the boundary situations and the analytical, simulated hydrogen solutions for case 3 (constant inflow temperature and variable outflow temperatures).

Table.2. Parameter for dual zone mode

Parameter	Value	Parameter	Value
a_{in}	0.0289	m_w	4.5
A_{in}	0.175929	M_{H_2}	2.0159e-3
c_p	14.615	R	8.314
c_v	10.316	T_0	300
c_w	10	T_∞	300
m_0	1	T_{w_0}	300
$\dot{m}_{in}$	0.0005	V	0.1508
$\dot{m}_{out}$	-0.0005		

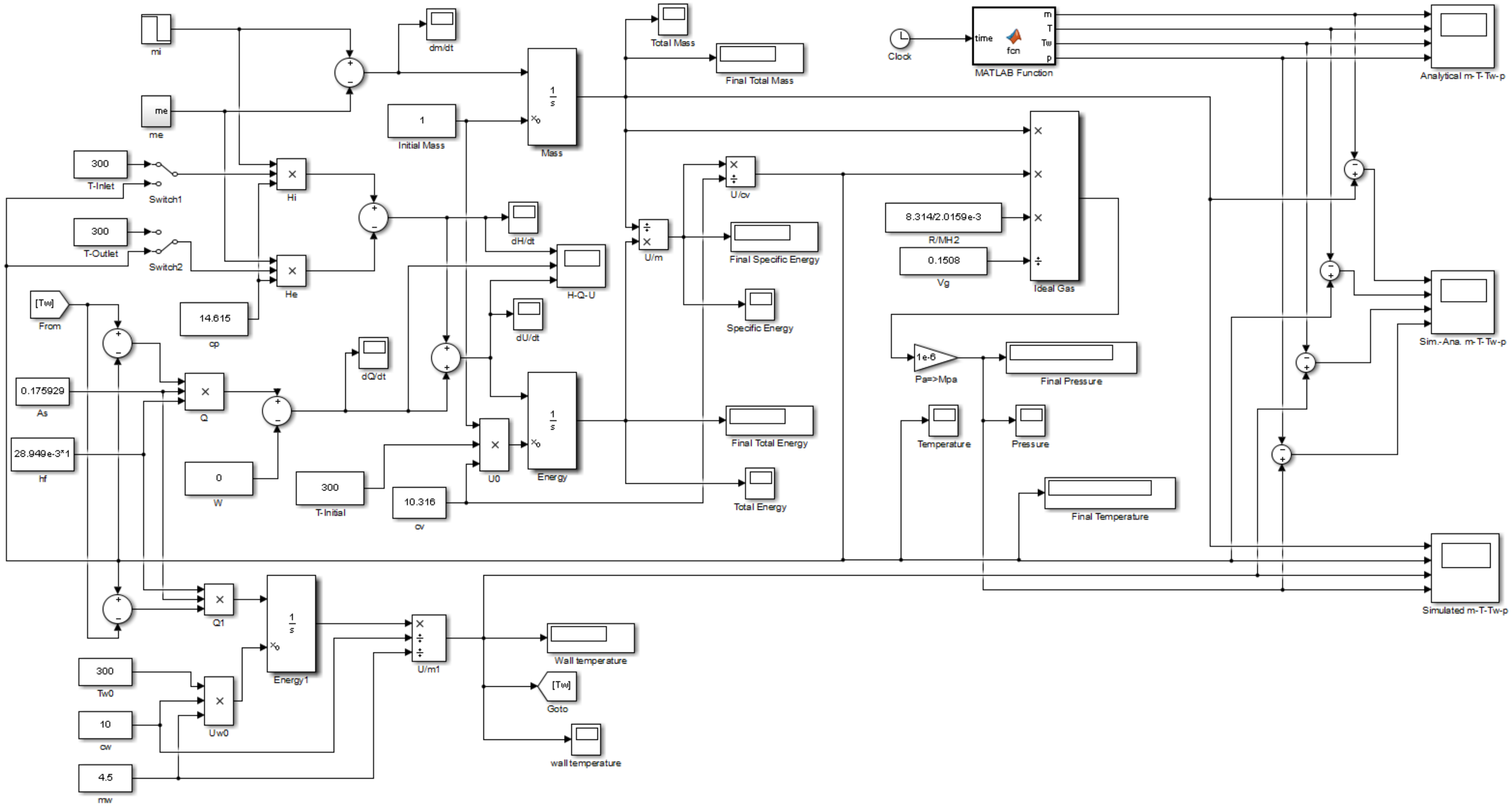

Figure.1 Matlab/Simulink model with function of analytical solution.

Table.1 Summary of thermodynamic equations and solutions in charge-discharge cycle.

Items	Charge/discharge processes with constant inflow/outflow temperatures	Charge/discharge processes with variable inflow/outflow temperatures	Dormancy processes after charge or discharge
Mass balance equation, kg/s	$\frac{dm}{dt} = \dot{m}$		$\frac{dm}{dt} = 0$
Solution of mass, kg	$m = m_0 + \dot{m}t$		$m = m_0$
Energy balance equation, W	$\frac{d(mu)}{dt} = \dot{m}h + A_{in}a_{in}(T_w - T)$ $\frac{d(m_w c_w T_w)}{dt} = A_{in}a_{in}(T - T_w)$		$\frac{d(mu)}{dt} = a_{\mathrm{in}}A_{\mathrm{in}}(T_w - T)$ $\frac{d(m_w c_w T_w)}{dt} = a_{in}A_{in}(T - T_w)$
Gas temperature rate, K/s	$\frac{dT}{dt} = \frac{\gamma T_\infty + \alpha(T_w - T) - T}{t^* + t}$	$\frac{dT}{dt} = \frac{\gamma T + \alpha(T_w - T) - T}{t^* + t}$	
Wall temperature rate, K/s	$\frac{dT_w}{dt} = \frac{T - T_w}{t_w^*}$		$\frac{dT_w}{dt} = AT_w + B$
Characteristic temperature, K	$T^* = \frac{\gamma T_\infty + \alpha T_w}{1 + \alpha}$	$T^* = \frac{\alpha T_w}{1 + \alpha - \gamma}$	
Temperature rate, K/s, use characteristic temperature	$\frac{dT}{dt} = (1 + \alpha)\frac{T^* - T}{t^* + t}$	$\frac{dT}{dt} = (1 + \alpha - \gamma)\frac{T^* - T}{t^* + t}$	
Solution of hydrogen temperature, K	$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1 + \tau}\right)^{1+\alpha}$	$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1 + \tau}\right)^{1+\alpha-\gamma}$	$T = T_0 + k\left(T_{w_0} - T_w\right)$
Solution of wall temperature, K	$\frac{T - T_w}{T - T_{w_0}} = e^{-\tau_w}$		$T_w = \left(T_{w_0} + \frac{B}{A}\right)e^{At} - \frac{B}{A}$
Adiabatic temperature, K	$\frac{T^* - T}{T^* - T_0} = \frac{1}{1 + \tau}$	$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1 + \tau}\right)^{1-\gamma}$	