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A Dual Zone Thermodynamic Model for Refueling Hydrogen Vehicles

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厚德博学 追求卓越

OUTLINE

- Introduction
- Thermodynamic model
- Analytical solutions
- Results and discussion
- Conclusion
- Acknowledgement

Introduction

- Compressed hydrogen gas cylinder is currently widely used to store the hydrogen due to its simplicity in tank structure and refueling process.

- For safety reason, the final gas temperature in the hydrogen tank during vehicle refueling must be controlled under a certain limit, e.g., 85°C.

- SAE J2601 standard describes the MC method which considers the heat capacity of the tank wall, but it uses single temperature for both hydrogen gas and tank wall.

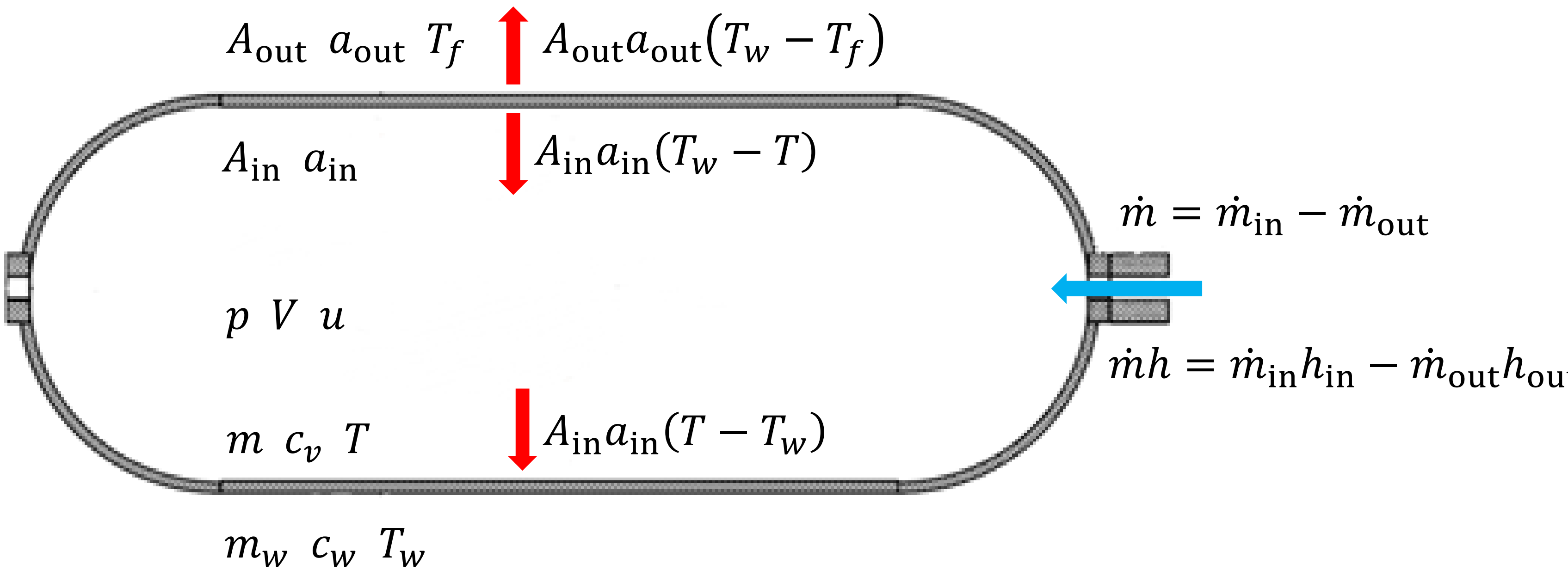
- Now we extend this model to dual zone and dual temperature model which includes hydrogen and tank wall.

Thermodynamic model

Sketch of hydrogen storage tank

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

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



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

Fig.1 Sketch of hydrogen storage tank

OUTLINE

Thermodynamic model

Mass and energy balance equation (I)

Hydrogen gas model:

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

Change of H_2 mass | Inflow mass rate | Outflow mass rate

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

Change of internal energy | Rate of inflow Enthalpy | Rate of outflow Enthalpy | Heat transfer from hydrogen gas to tank

Simplified form:

$$\boxed{\frac{dm}{dt} = \dot{m}}$$

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

Tank wall model:

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

Rate of internal energy | Heat transfer from hydrogen gas to tank | Heat transfer from ambient environment to tank

Supposing $a_{\text{out}} = 0$:

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

Thermodynamic model

Mass and energy balance equation (II)

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

$$\frac{d(mu)}{dt} = m\frac{du}{dx} + \dot{m}u$$

$$m = m_0 + \dot{m}t$$

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

Divided by $\dot{m}c_v$

Defining $t^* = m_0/\dot{m}$,
$\gamma = c_p/c_v$,
$\alpha = \frac{A_{in}a_{in}}{c_v\dot{m}}$

$$u = c_vT$$

$$h = c_pT_\infty$$

$$\boxed{(t^* + t)\frac{dT}{dt} + T = \gamma T_\infty + \alpha(T_w - T)}$$

OUTLINE

Analytical solution

Wall temperature

Energy balance for tank wall during charge/discharge process

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

Defining $t_w^* = \frac{m_w c_w}{a_{in} A_{in}}$

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

Supposing T is constant

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

Temperature of tank wall T_w can be written in the form of "rule of mixture":

$$T_w = f_w T_{w_0} + (1 - f_w) T \quad \text{where} \quad f_w = e^{-\tau_w}$$

OUTLINE

Analytical solution

Constant inflow/outflow temperature

$$(t^* + t)\frac{dT}{dt} + T = \gamma T_\infty + \alpha(T_w - T)$$

$$\frac{dT}{dt} = (1+\alpha)\frac{T^* - T}{t^* + t}$$ where $T^* = \frac{\gamma T_\infty + \alpha T_w}{1+\alpha}$

Solution when supposing T_w is constant:

$$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1+\tau}\right)^{1+\alpha}$$ where $\tau = t/t^*$

In the form of "rule of mixture":

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

OUTLINE

Analytical solution

Variable inflow/outflow temperature

$$(t^* + t)\frac{dT}{dt} + T = \gamma T_\infty + \alpha(T_w - T)$$

$$\frac{dT}{dt} = (1+\alpha)\frac{T^* - T}{t^* + t} \qquad \text{where } T^* = \frac{\alpha}{1+\alpha-\gamma} T_w$$

Solution when supposing T_w is constant:

$$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1+\tau}\right)^{1+\alpha} \qquad \text{where } \tau = t/t^*$$

In the form of "rule of mixture":

$$T = f_g T_0 + (1 - f_g)T^* \qquad \text{where } f_g = \left(\frac{1}{1+\tau}\right)^{1+\alpha-\gamma}$$

Analytical solution

Constant inflow/outflow temperature

Hydrogen gas: $T = f_g T_0 + \left(1 - f_g\right) T^*$

Tank wall: $T_w = f_w T_{w_0} + (1 - f_w) T$

Noting $T^* = \frac{\gamma T_\infty + \alpha T_w}{1+\alpha}$ makes the algebraic equations coupled, they can be solved simultaneously.

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

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

OUTLINE

Analytical solution

Variable inflow/outflow temperature

Hydrogen gas: $T = f_g T_0 + (1 - f_g) T^*$

Tank wall: $T_w = f_w T_{w0} + (1 - f_w) T$

Noting $T^* = \frac{\alpha T_w}{1+\alpha-\gamma}$ makes the algebraic equations coupled, they can be solved simultaneously.

$$T = \frac{f_g T_0 + \frac{\alpha}{1+\alpha-\gamma} f_w (1 - f_g) T_{w0}}{1 - \frac{\alpha}{1+\alpha-\gamma}(1 - f_g)(1 - f_w)}$$

$$T_w = \frac{f_w T_{w0} + f_g (1 - f_w) T_0}{1 - \frac{\alpha}{1+\alpha-\gamma}(1 - f_g)(1 - f_w)}$$

Analytical solution

Temperature during dormancy

Hydrogen gas: $$\frac{d(mc_vT)}{dt} = a_{in}A_{in}(T_w - T)$$

Tank wall: $$\frac{d(m_wc_wT_w)}{dt} = a_{in}A_{in}(T - T_w)$$

Divided the latter equation by former one

$$\frac{mc_v}{m_wc_w}\frac{dT}{dT_w} = -1 \quad \Rightarrow \quad T = T_0 + k\left(T_{w_0} - T_w\right)$$

Then

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

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

where $A = -(k+1)/t_w^*$

$B = \left(T_0 + kT_{w_0}\right)/t_w^*$

$k = m_wc_w/(mc_v)$

OUTLINE

Analytical solution

Summary of equations and solutions (I)

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

Items	Charge/discharge processes	Dormancy processes
Mass balance equation, kg/s	$\frac{dm}{dt} = \dot{m}$	$\frac{dm}{dt} = 0$
Hydrogen mass, kg	$m = m_0 + \dot{m}t$	$m = m_0$
Energy balance equations, W	$\frac{d(mu)}{dt} = \dot{m}h + A_{in}a_{in}(T_w - T)$ $\frac{d(m_w c_w T_w)}{dt} = A_{in}a_{in}(T - T_w)$	$\frac{d(mu)}{dt} = a_{\mathrm{in}}A_{\mathrm{in}}(T_w - T)$ $\frac{d(m_w c_w T_w)}{dt} = a_{in}A_{in}(T - T_w)$
Rate of wall temperature, K/s	$\frac{dT_w}{dt} = \frac{T - T_w}{t_w^*}$	$\frac{dT_w}{dt} = AT_w + B$
Solution of wall temperature, K	$\frac{T - T_w}{T - T_{w0}} = e^{-\tau_w}$	$T_w = \left(T_{w0} + \frac{B}{A}\right)e^{At} - \frac{B}{A}$
Hydrogen temperature, K	See Table 2	$T = T_0 + k\left(T_{w0} - T_w\right)$

OUTLINE

Analytical solution

Summary of equations and solutions (II)

Table 2 Charge/discharge processes with different inflow/outflow temperatures

Items	Constant inflow/outflow temperatures	Variable inflow/outflow temperatures
Rate of hydrogen temperature, K/s	$\frac{dT}{dt} = \frac{\gamma T_\infty + \alpha(T_w - T) - T}{t^* + t}$	$\frac{dT}{dt} = \frac{\gamma T + \alpha(T_w - T) - T}{t^* + t}$
Characteristic temperature, K	$T^* = \frac{\gamma T_\infty + \alpha T_w}{1 + \alpha}$	$T^* = \frac{\alpha T_w}{1 + \alpha - \gamma}$
Rate of hydrogen temperature, K/s	$\frac{dT}{dt} = (1 + \alpha)\frac{T^* - T}{t^* + t}$	$\frac{dT}{dt} = (1 + \alpha - \gamma)\frac{T^* - T}{t^* + t}$
Solution of hydrogen temperature, K	$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1 + \tau}\right)^{1+\alpha}$	$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1 + \tau}\right)^{1+\alpha-\gamma}$
Adiabatic charging temperature, K	$\frac{T^* - T}{T^* - T_0} = \frac{1}{1 + \tau}$	$\frac{T^* - T}{T^* - T_0} = \left(\frac{1}{1 + \tau}\right)^{1-\gamma}$

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Results and Discussion

Matlab/Simulink Model

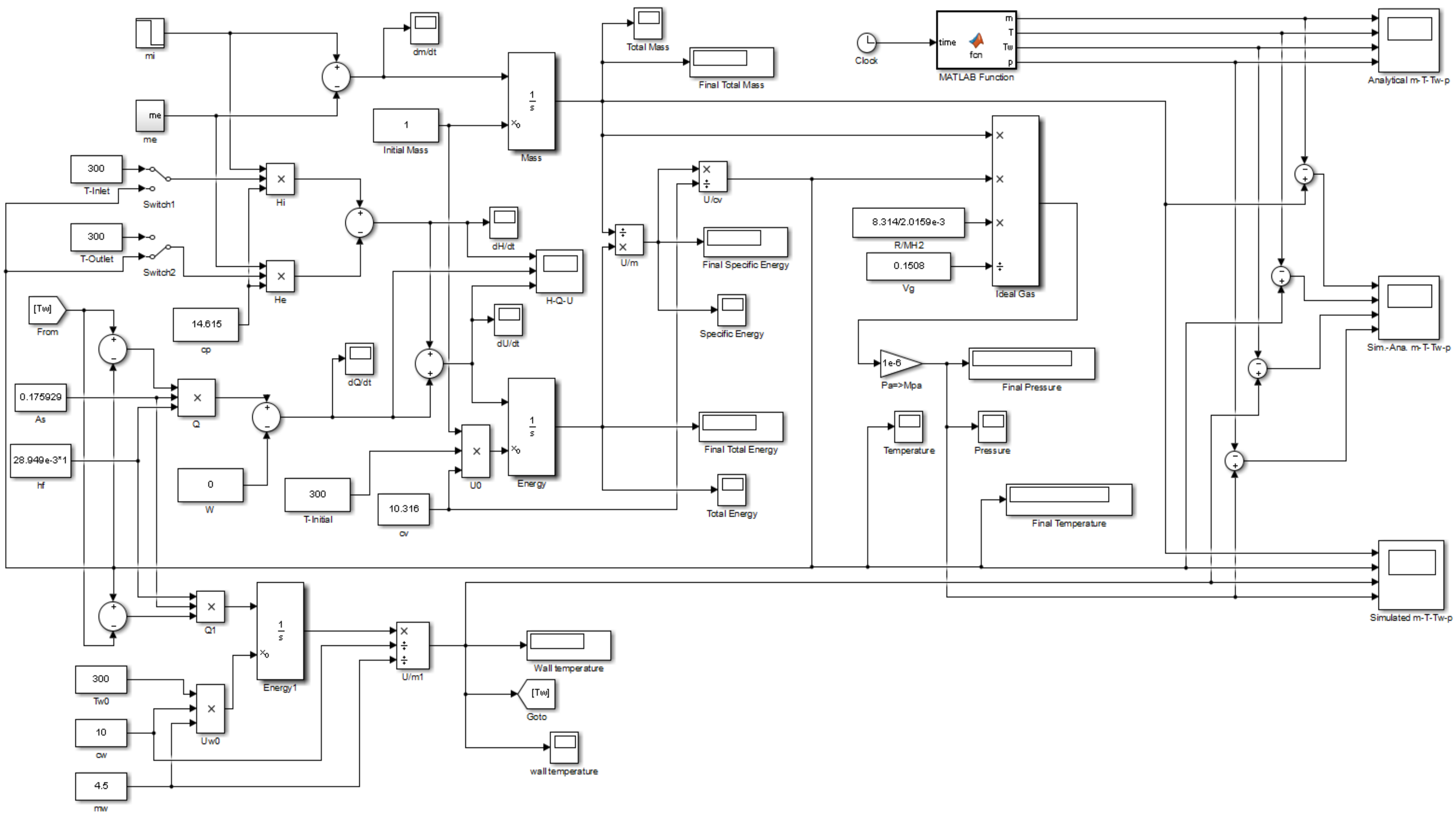

Fig.2 Matlab/Simulink model with function of analytical solution.

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Results and Discussion

Parameter values

Table 3 Parameters used in the simulation.

Parameter	Definition	Value	Parameter	Definition	Value
a_{in}	Heat transfer coefficient of inner surface,W/m²/K	0.0289	m_w	Mass of tank wall, kg	4.5
A_{in}	Inner surface area of tank, m²	0.175929	m_0	Initial hydrogen mass in tank, kg	1
c_p	Constant pressure specific heat, kJ/kg/K	14.615	R	Universal gas constant, R=8.314J/K/mol	8.314
c_v	Constant volume specific heat, kJ/kg/K	10.316	T_0	Initial temperature in tank, K	300
c_w	Specific heat of tank wall, kJ/kg/K	10	T_∞	Hydrogen inflow temperature, K	300
$\dot{m}_{in}$	Hydrogen mass inflow rate, kg/s	0.0005	T_{w0}	Initial temperature of tank wall, K	300
$\dot{m}_{out}$	Hydrogen mass outflow rate, kg/s	-0.0005	V	Volume of tank, m³	0.1508

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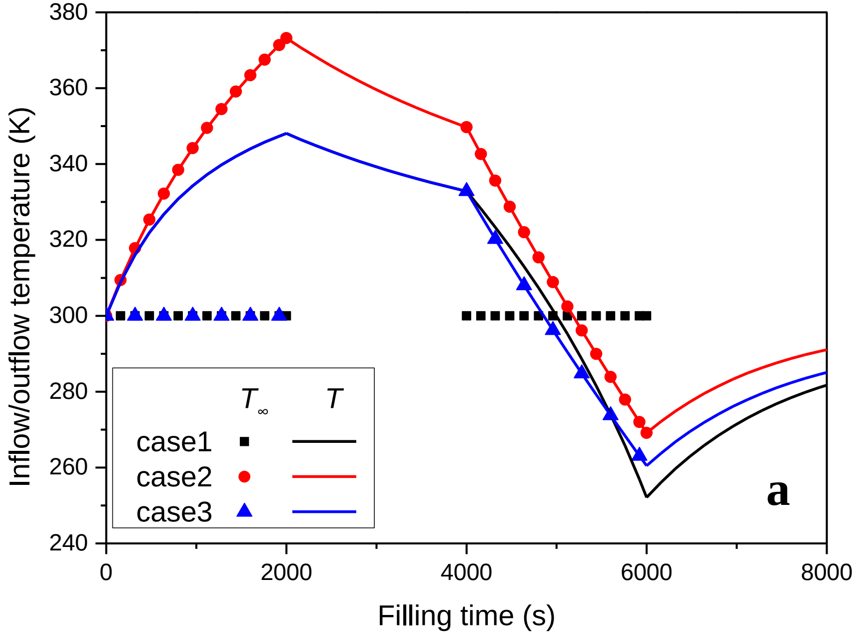
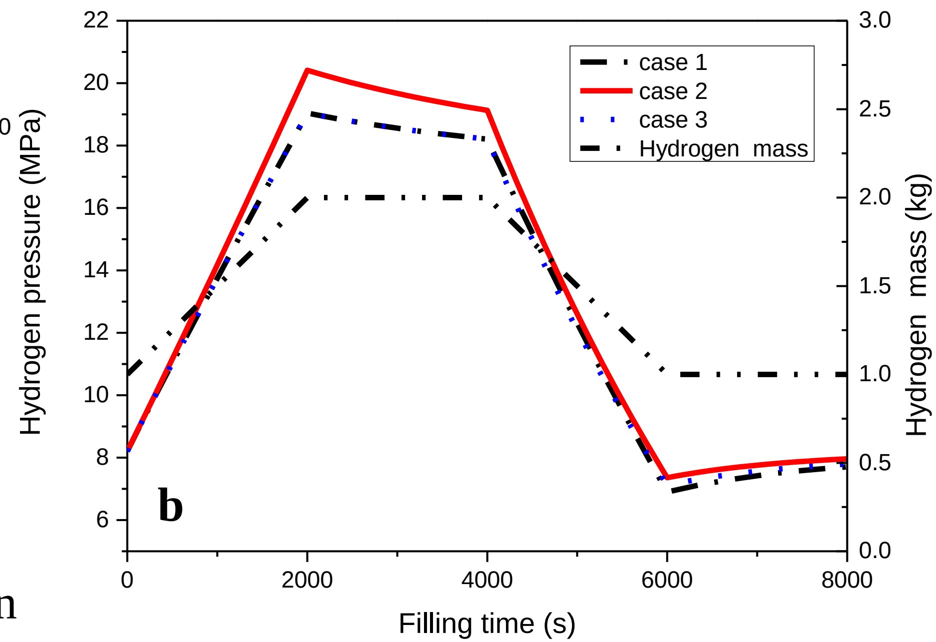
Results and Discussion

Analytical solutions for three cases (I)



Case 1: Constant inflow/outflow temperatures.
Case 2: Variable inflow/outflow temperatures
Case 3: Constant inflow temperature and variable outflow temperature.



Inflow temperature in case 2 is higher than it in other cases and more energy is carried into tank. As a results, pressure in case 2 is higher than it in other cases.

Fig.3 Comparison of (a) inflow/outflow temperature and (b) pressure and hydrogen mass under different inflow/outflow temperatures

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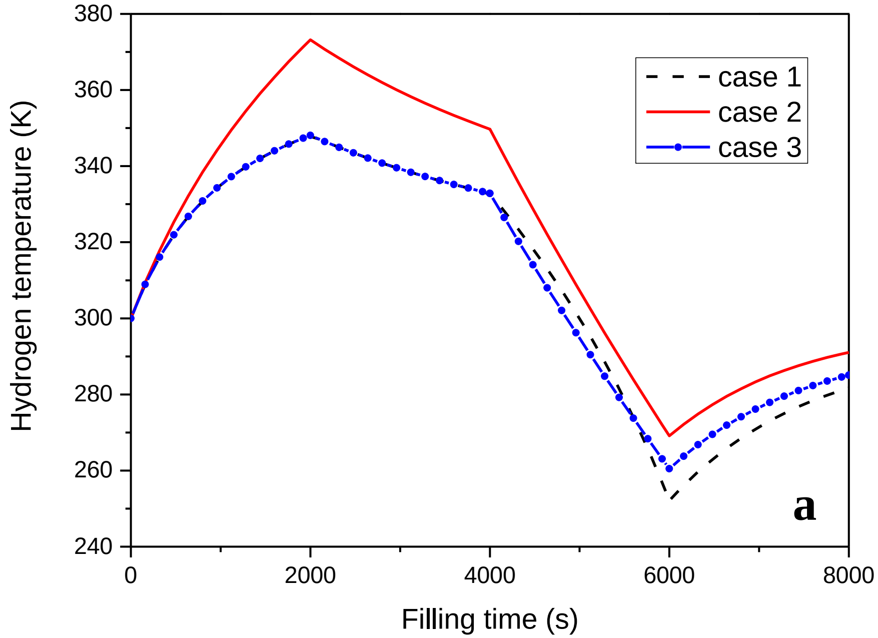
Results and Discussion

Analytical solutions for three cases (II)



Case 3: It is the most practical situation and can be used as the reference case.
Case 2: Higher inflow temperature causes higher enthalpy entering the tank, and causes higher gas temperature and wall temperature.
Case 1: The constant outflow temperature (300K) is almost the average of variable outflow temperature. So their temperature curves are very close.

Case 1: Constant inflow/outflow temperatures.
Case 2: Variable inflow/outflow temperatures.
Case 3: Constant inflow temperature and variable outflow temperature.

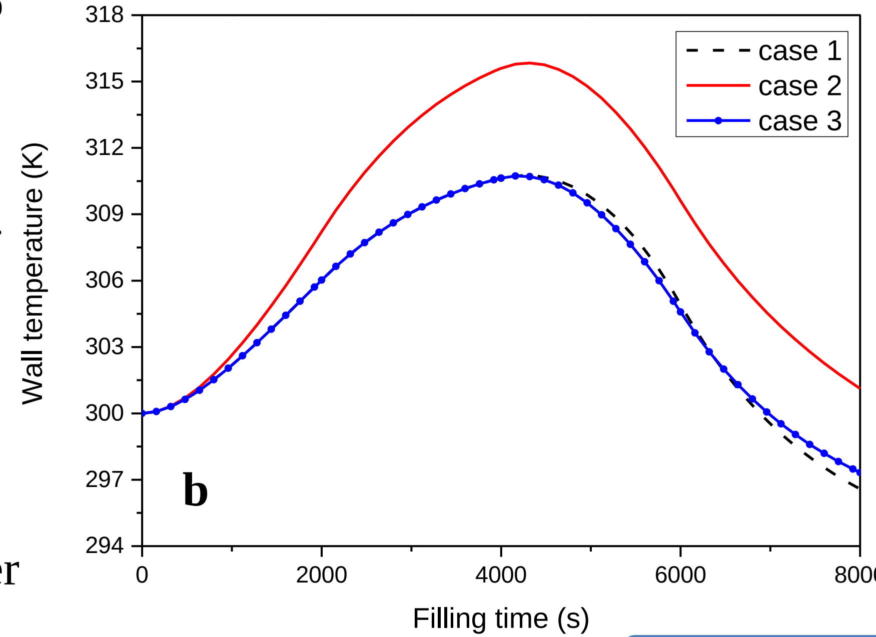


Fig.4 Comparison of (a) hydrogen gas temperature and (b) wall temperature under different inflow/outflow temperatures

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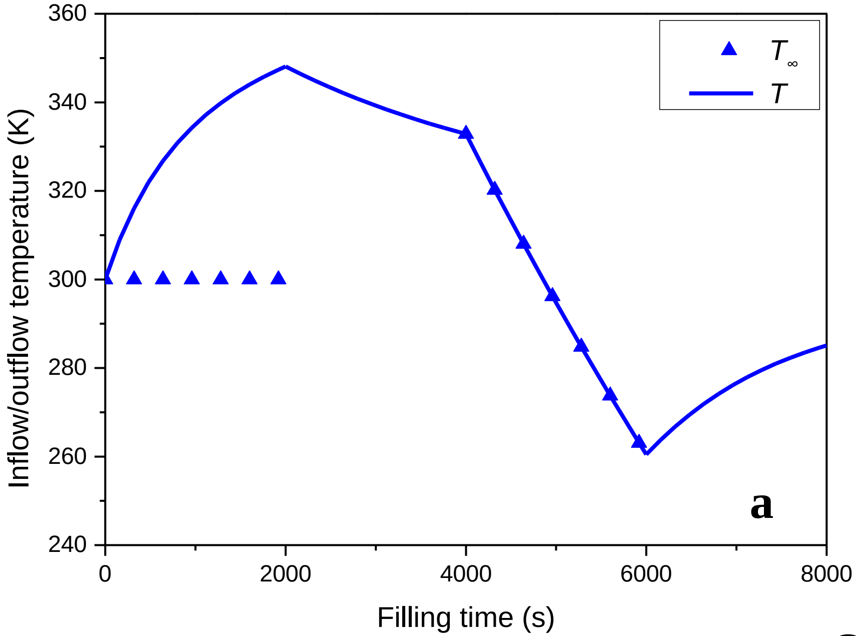
Results and Discussion

Comparison between analytical and simulated solutions (I)



Case 3: Constant inflow temperature and variable outflow temperature.

Analytical solution agree well with numerical solution in hydrogen mass and pressure.

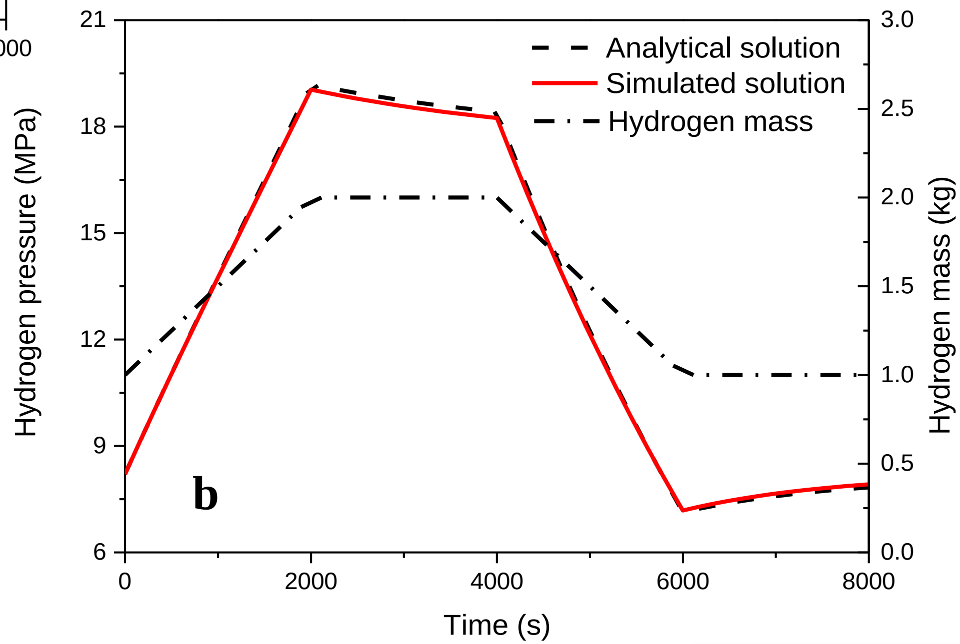
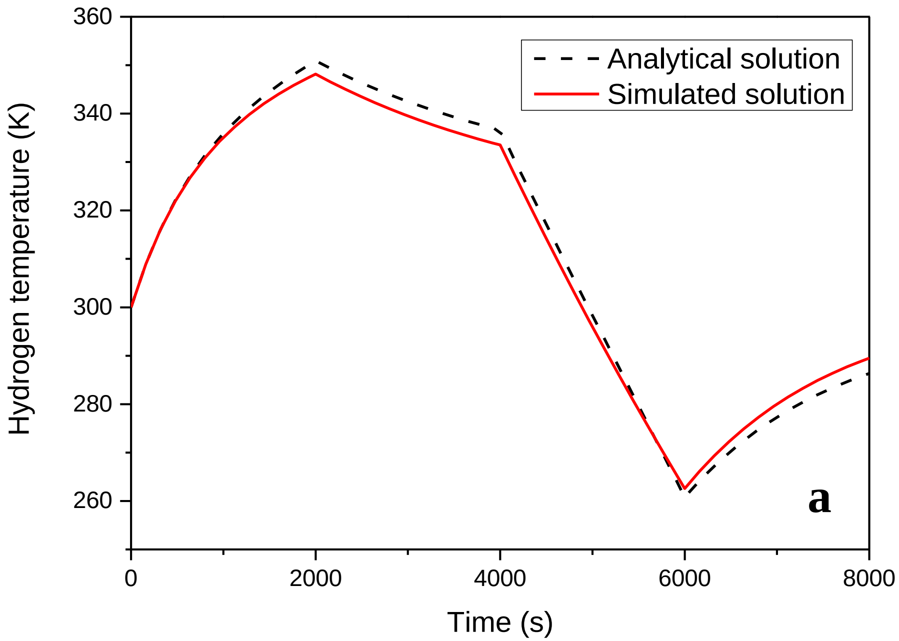


Fig.5 Comparison of (a) inflow/ outflow temperature and (b) pressure and hydrogen mass between analytical and simulated solutions

Results and Discussion

Comparison between analytical and simulated solutions (II)



Case 3: Constant inflow temperature and variable outflow temperature.

As for the hydrogen temperature, the difference between analytical solution and numerical solution is slight. Effort can be made for obtain more precise analytical solution.

As for the wall temperature, analytical solution increases fast and reaches a higher peak than simulated solution during charging and decreases fast and reaches a lower value.

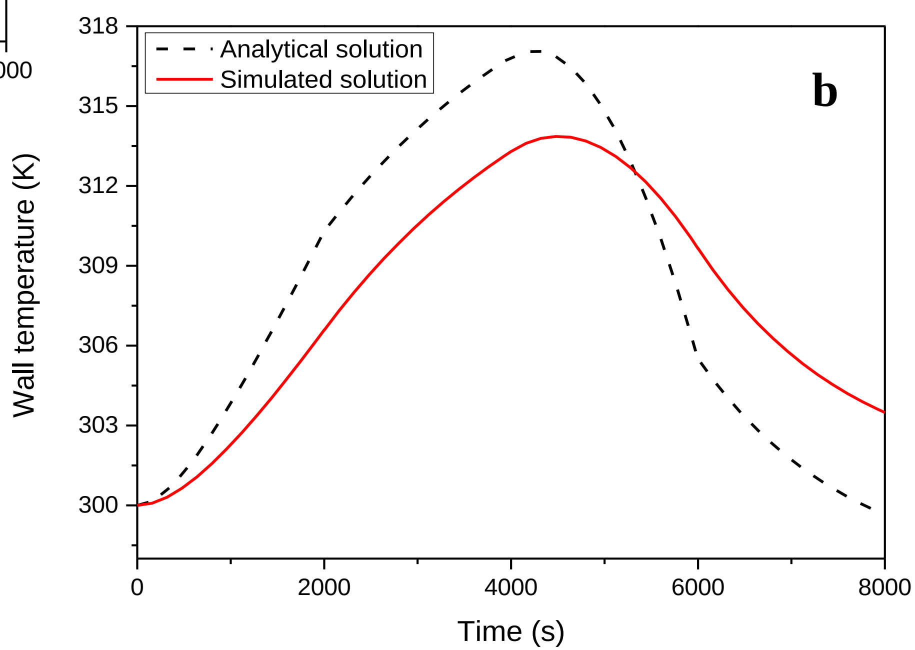
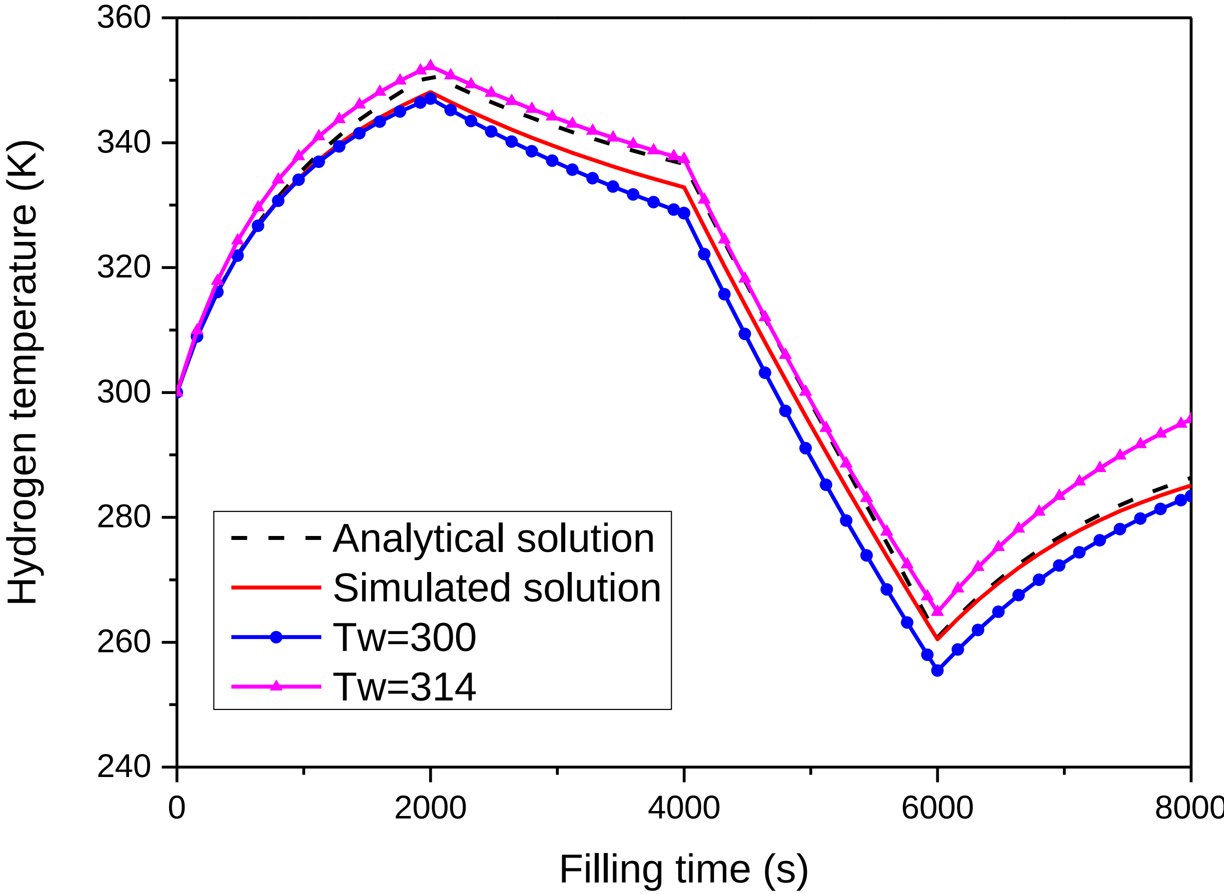


Fig.6 Comparison of (a) hydrogen gas temperature and (b) wall temperature between analytical and simulated solutions

OUTLINE

Results and Discussion

Comparison between analytical and simulated solutions (III)



Wall temperature is set as 300K and 314K in two cases, which are minimum and maximum wall temperature in simulated solution, respectively.

The dual zone model is simplified to be single zone model in the two cases.

Analytical solution and simulated solution of the case 3 are between the two fixed bound situations.

Fig.7 Comparison of temperature between analytical and numerical solutions for different boundary conditions

Conclusions

- Thermodynamic behaviors for charging-discharging cycle of compressed hydrogen system is described by a dual zone thermodynamic model.

- 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. 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 Matlab/Simulink, which can be used to compare with the analytical solutions and to improve our model.

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Thanks for your attentions!

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