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Improvement of MC Method in SAE J2601 Hydrogen Refuelling Protocol Using Dual-Zone Dual-Temperature Model

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Outline

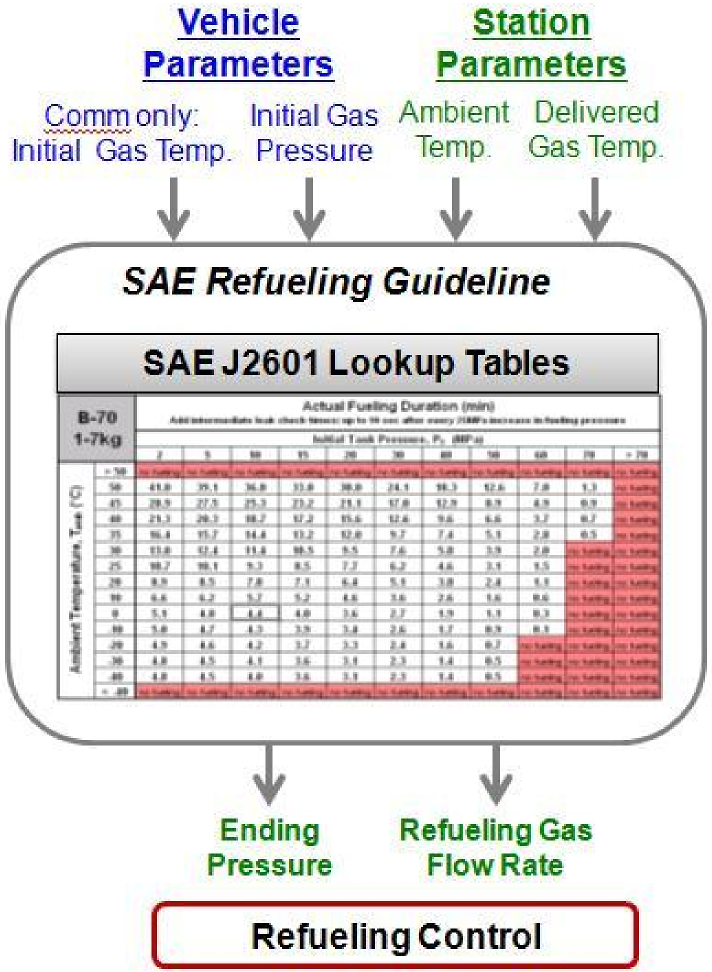
- Introduction
- Model Description and Validation
- Improvements for MC method
- Results and Discussion
- Conclusions

Introduction

Inputs

Station Dispenser Type

- •T40 Station H2@ -40˚C
- •T30 Station H2@ -30˚C
- •T20- Station H2@ -20˚C



Vehicle Parameters

Commonly: Initial Gas Temp.

Initial Gas Pressure

Station Parameters

Ambient Temp.

Delivered Gas Temp.

SAE Refueling Guideline

SAE J2601 Lookup Tables

Ending Pressure

Refueling Gas Flow Rate

Refueling Control

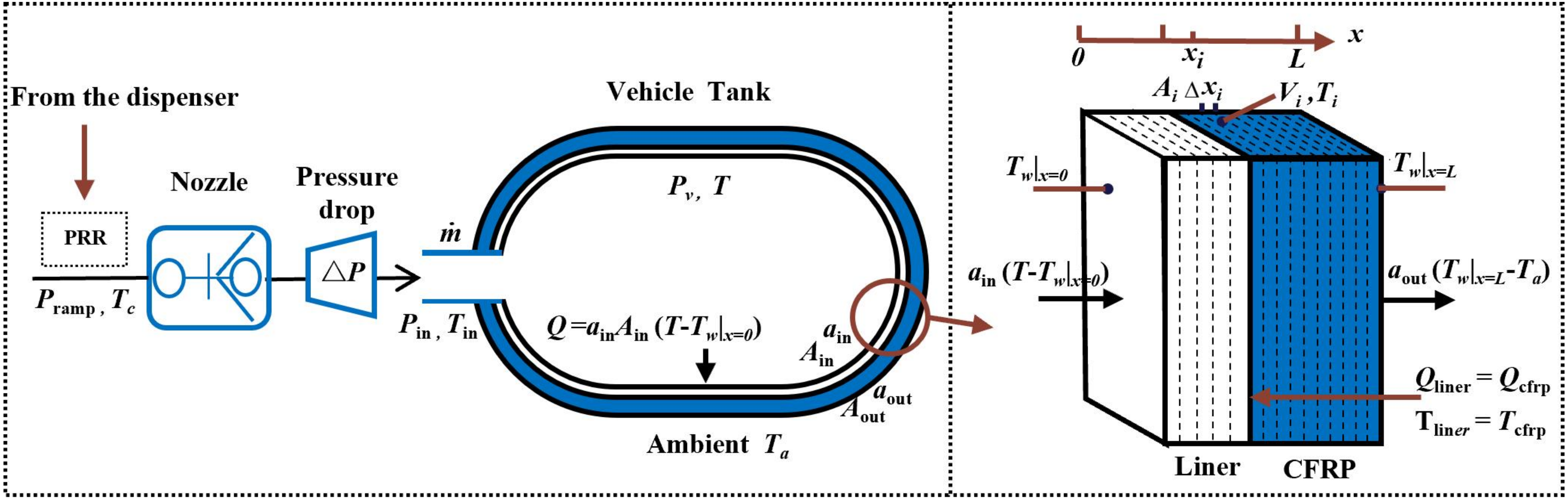
[*]https://www.sae.org/news/2014/07/hydrogen-fueling-protocol-spelled-out-in-new-sae-international-j2601-standard

- ● In order to refuel hydrogen fuel cell vehicles quickly and safely, two **refueling methods** have been implemented in SAE J2601, include **lookup table method** and **MC method**.
- ● Both methods control the **refueling gas flow rate** and **ending pressure** according to the **vehicle parameters** and **station parameters**.
- ● **Refueling gas flow rate is reflected by pressure ramp rate (PRR).**
- ● This article mainly improves the **calculation method of the ending pressure** in MC method. Accurate estimation for final hydrogen temperature, ending pressure and final SOC to control the refuelling is **safer**.

Model Description

0D1D hydrogen filling model

- This Figure shows a **simplified hydrogen filling model** from the dispenser to the vehicle tank.
- **Hydrogen** inside tank is lumped parameter model **(0D)**, and tank wall is represented by one-dimensional model **(1D)**.
- This 0D1D model is used to **generate simulation data to fit the correction factor** and **verify the modified MC method**.



Model Description

Mathematical equations for 0D1D model

- **Mass and energy conservation for hydrogen inside tank**

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

$$\frac{d(mu)}{dt} = \dot{m}_{\text{in}}\, h_{\text{in}} - \dot{m}_{\text{out}}\, h_{\text{out}} + \dot{Q}$$

- **Heat transfer equation for one-dimensional tank wall**

$$\lambda_w \frac{\partial^2 T_w}{\partial x^2} = \rho_w c_w \frac{\partial T_w}{\partial t}$$

- **Boundary conditions of inner and outer surfaces of tank**

$$-\lambda_w \frac{\partial T_w}{\partial x}\bigg|_{x=0} = \alpha_{\text{in}}\left(T - T_w|_{x=0}\right)$$

$$-\lambda_w \frac{\partial T_w}{\partial x}\bigg|_{x=L} = \alpha_{\text{out}}\left(T_w|_{x=L} - T_a\right)$$

- **Heat transfer coefficient between hydrogen and inner wall**

$$a_{\text{in}} = \frac{0.14\lambda \mathrm{Re}_{d_{\text{in}}}^{0.67}}{D_{\text{in}}}$$

- **Heat transfer coefficient between outer wall and ambient**

$$a_{\text{out}} = \frac{\lambda_a \, \mathrm{Pr}_a^{0.4}\left(0.4\mathrm{Re}_{D_{\text{out}}}^{0.5} + 0.06\mathrm{Re}_{D_{\text{out}}}^{2/3}\right)}{D_{\text{out}}}$$

- **Pressure drop**

$$\Delta P = k_p \frac{\dot{m}^2}{\rho}$$

Model Description

Control process of MC method—Refueling gas flow rate ⇒ **reflected by the pressure ramp rate (PRR).**

- Calculate **mass average temperature (MAT)** of the inlet flow.
- Calculate the MAT for control (**MATC**) based on three rules.
- Calculate final filling time t_{final} using MATC.
- Calculate **PRR** using t_{final}.

$$\mathrm{MAT}_{(j)} = \frac{\sum_1^j \left(m_{(j)} - m_{(j-1)}\right) \times 0.5\left(T_{(j)} + T_{(j-1)}\right)}{\sum_1^j \left(m_{(j)} - m_{(j-1)}\right)}$$

(1) Rule 1: if $t(j) \leq 30$ s, $\mathrm{MATC}_{(j)} = \mathrm{MAT}_{\text{exp}}$

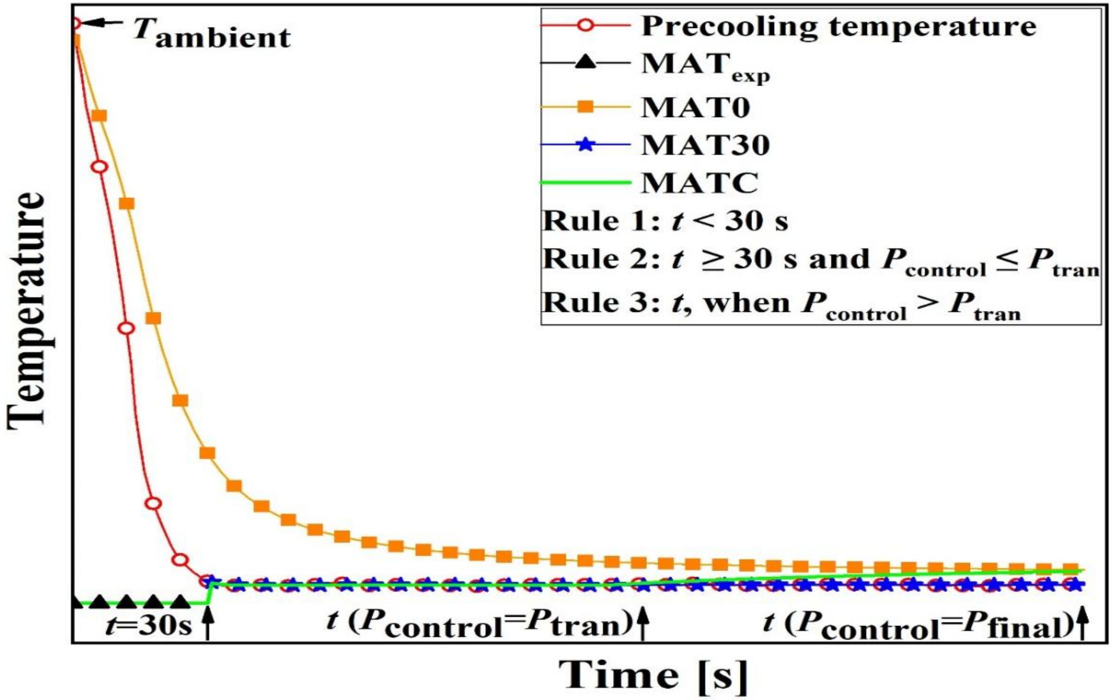
(2) Rule 2: if $t(j) > 30$ s and $P_{\text{control}(j)} \leq P_{\text{trans}}$, $\mathrm{MATC}_{(j)} = \mathrm{MAT30}_{(j)}$

(3) Rule 3: if $P_{\text{control}(j)} > P_{\text{trans}}$,

$$\mathrm{MATC}_{(j)} = \mathrm{MAT30}_{(j)} \left(\frac{P_{\text{final}} - P_{\text{control}(j)}}{P_{\text{final}} - P_{\text{trans}}}\right) + \mathrm{MAT0}_{(j)} \left(1 - \frac{P_{\text{final}} - P_{\text{control}(j)}}{P_{\text{final}} - P_{\text{trans}}}\right)$$

$$t_{\text{final}(j)} = a \times \mathrm{MATC}_{(j)}{}^3 + b \times \mathrm{MATC}_{(j)}{}^2 + c \times \mathrm{MATC}_{(j)} + d$$

$$\mathrm{PRR}_{(j)} = \frac{P_{\text{final}} - P_{\text{ramp}(j)}}{t_{\text{final}(j)}\left(\frac{P_{\text{final}} - P_{\text{initial}}}{P_{\text{final}} - P_{\text{min}}}\right) - t_{(j)}}$$



Model Description

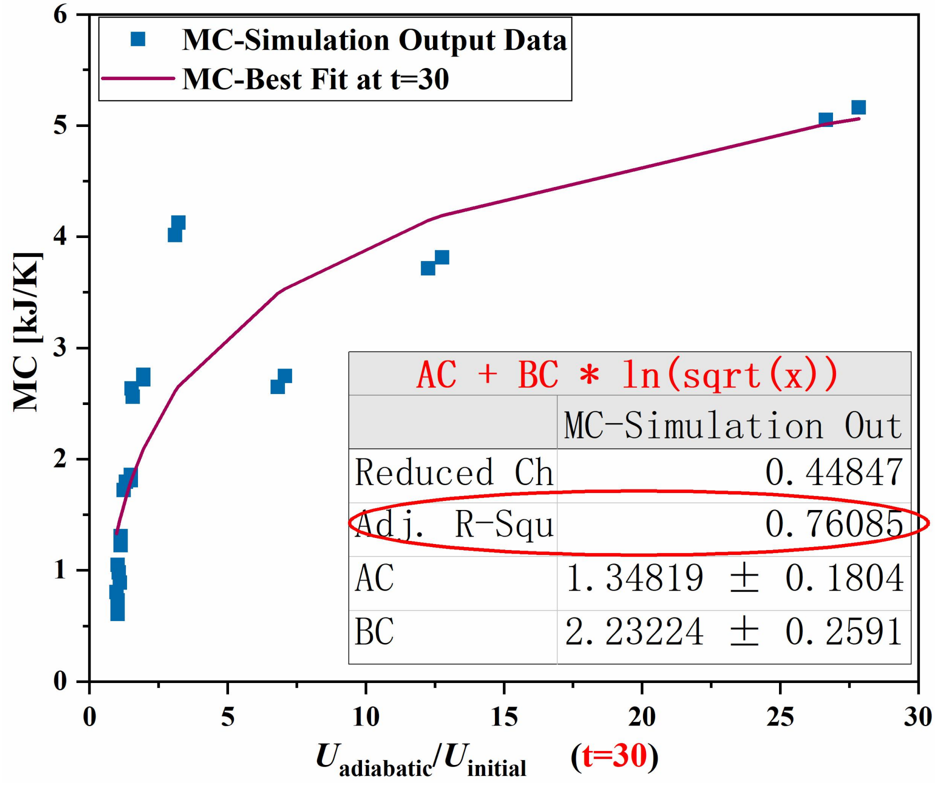
Control process of MC method—Ending Pressure

- The analytical solution of final hydrogen temperature is used to determine ending pressure (target pressure).
- Data from 0D1D model are used to fit the MC expression.
- Left figure is the result of fitting the first term.
- Right figure is the result of fitting the second term.

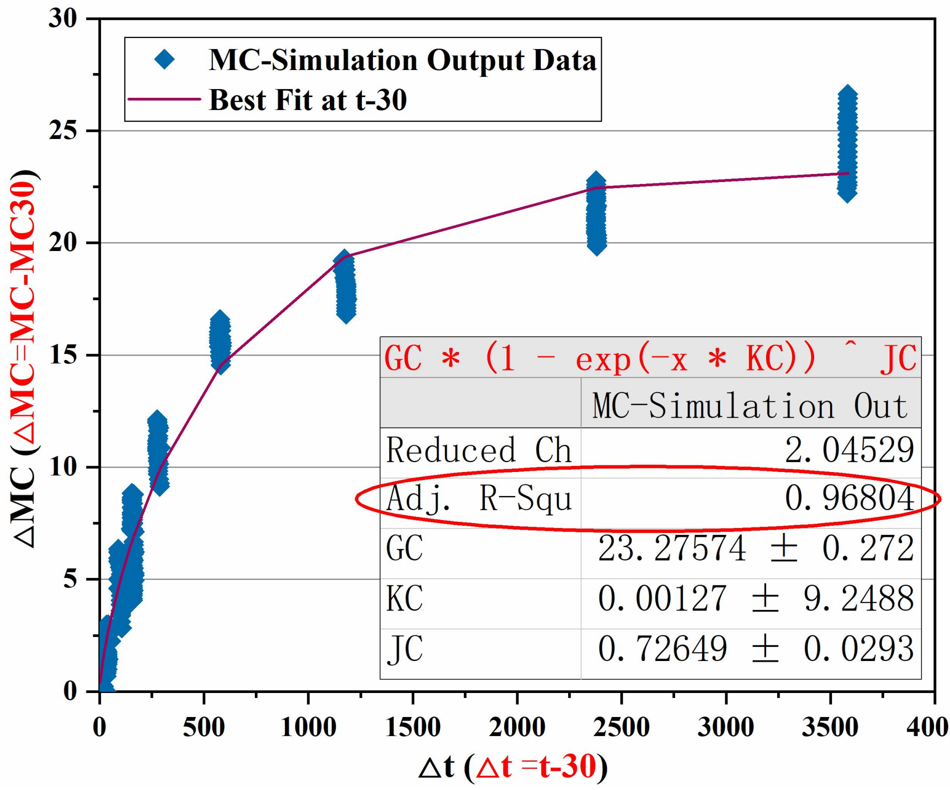
$$T_{\text{final}} = \frac{m_{\text{final}} c_v T_{\text{adiabatic}} + \mathbf{MC}\, T_{\text{initial}}}{\mathbf{MC} + m_{\text{final}} c_v}$$

$$P_{\text{target}} = f(T_{\text{final}},\ \text{SOC}_{\text{target}})$$

$$\mathbf{MC} = \text{AC} + \text{BC}\ln\left(\frac{U_{\text{adiabatic}}}{U_{\text{initial}}}\right)^{1/2} + \text{GC}\left(1 - e^{-\text{KC}\Delta t}\right)^{\text{JC}}$$



AC + BC * ln(sqrt(x))	
	MC-Simulation Out
Reduced Ch	0.44847
Adj. R-Squ	0.76085
AC	1.34819 ± 0.1804
BC	2.23224 ± 0.2591

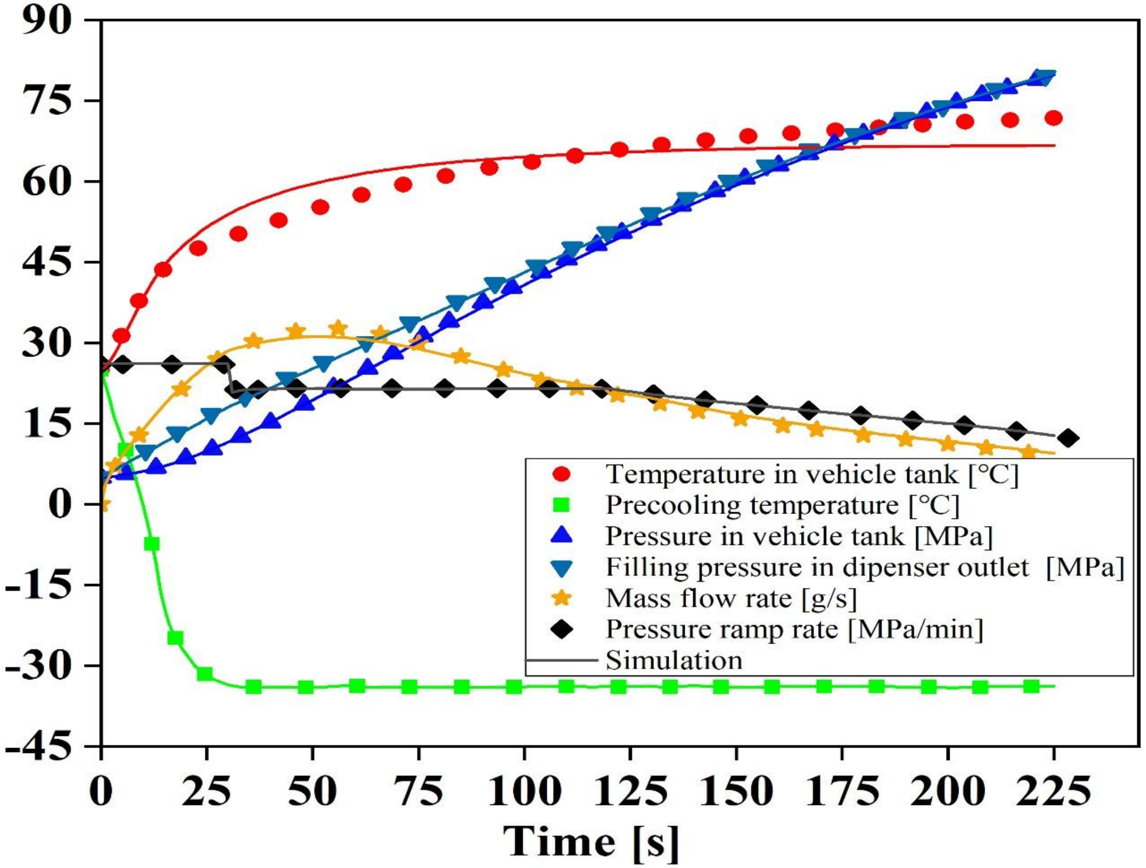


GC * (1 - exp(-x * KC)) ^ JC	
	MC-Simulation Out
Reduced Ch	2.04529
Adj. R-Squ	0.96804
GC	23.27574 ± 0.272
KC	0.00127 ± 9.2488
JC	0.72649 ± 0.0293

Model Validation

			Model validation	Improvements for MC method
		Units	70 MPa Type IV [3]	1kg 70 MPa Type III [1]
Geometry	Internal gas volume	liter	129	25
	Total external length	mm	722	835
	Internal liner surface area	m^2	1.3	0.5
	External/Internal diameter	mm	600/513	240/200
	Liner/CFRP wall thickness	mm	5/38.3	3.25/16.7
	Liner/CFRP mass	kg	6.1/72.4	4.7/14.9
Properties	Liner/CFRP density	kg/m^3	975/1550	2700/1494
	Liner/CFRP thermal conductivity	W/m/K	0.3/0.3	164/0.74
	Liner/CFRP specific heat capacity	J/kg/K	1000/500	1106/1120

- These model parameters are shown in the left table.
- PRR (black diamond) changes dynamically in three stages according to the three rules.
- The hydrogen mass flow rate (yellow star) agrees very well.
- The pressure (blue triangle) and temperature (red circle) of hydrogen agree well.



[1] Society of Automotive Engineers (SAE)., SAE J2601 (2020): Fueling protocols for light duty gaseous hydrogen surface vehicles, https://www.sae.org/standards/content/j2601_202005/.

[3] Reddi, K. and Elgowainy, A., Impact of hydrogen SAE J2601 fueling methods on fueling time of light-duty fuel cell electric vehicles, Int J Hydrogen Energy, 42, No. 26, 2017, pp. 16675-16685.

Improvements for MC method

Ending pressure determined by dual-zone single-temperature model in original MC method

Thermodynamic energy conservation during a refueling time of t_{initial} - t_{final}:

Hydrogen energy is transferred to the tank wall (assuming that the outer wall of the tank is **adiabatic**):

$m_{\text{final}}c_v(T_{\text{adiabatic}} - \boldsymbol{T}_{\textbf{final}}) = \text{MC}(\boldsymbol{T}_{\boldsymbol{w}\textbf{final}} - T_{\text{initial}})$

+

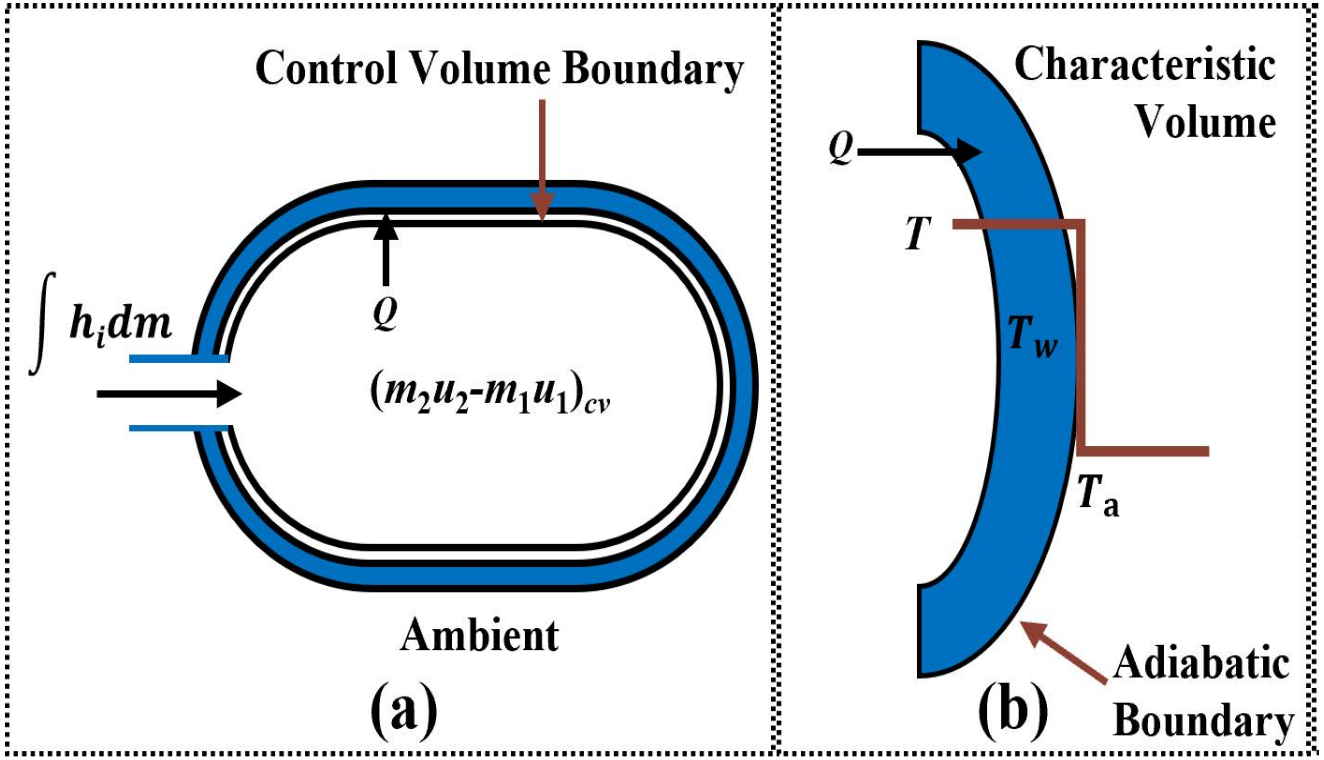
The original MC method assumes that: $\boldsymbol{T}_{\textbf{final}} = \boldsymbol{T}_{\boldsymbol{w}\textbf{final}}$

⇩

$$\boldsymbol{T}_{\textbf{final}} = \frac{m_{\text{final}}c_v T_{\text{adiabatic}} + \textbf{MC}T_{\text{initial}}}{\textbf{MC} + m_{\text{final}}c_v}$$

⇩

$$\boldsymbol{P}_{\textbf{target}} = f(\boldsymbol{T}_{\textbf{final}}, \ \text{SOC}_{\text{target}})$$



Improvements for MC method

Ending pressure determined by dual-zone dual-temperature model in modified MC method

Thermodynamic energy conservation during a refueling time of t_{initial} - t_{final}:

Hydrogen energy is transferred to the tank wall (assuming that the outer wall of the tank is **adiabatic**):

$$m_{\text{final}} c_v (T_{\text{adiabatic}} - \boldsymbol{T}_{\textbf{final}}) = m_w c_w (\boldsymbol{T}_{\textbf{wfinal}} - T_{\text{initial}})$$

+

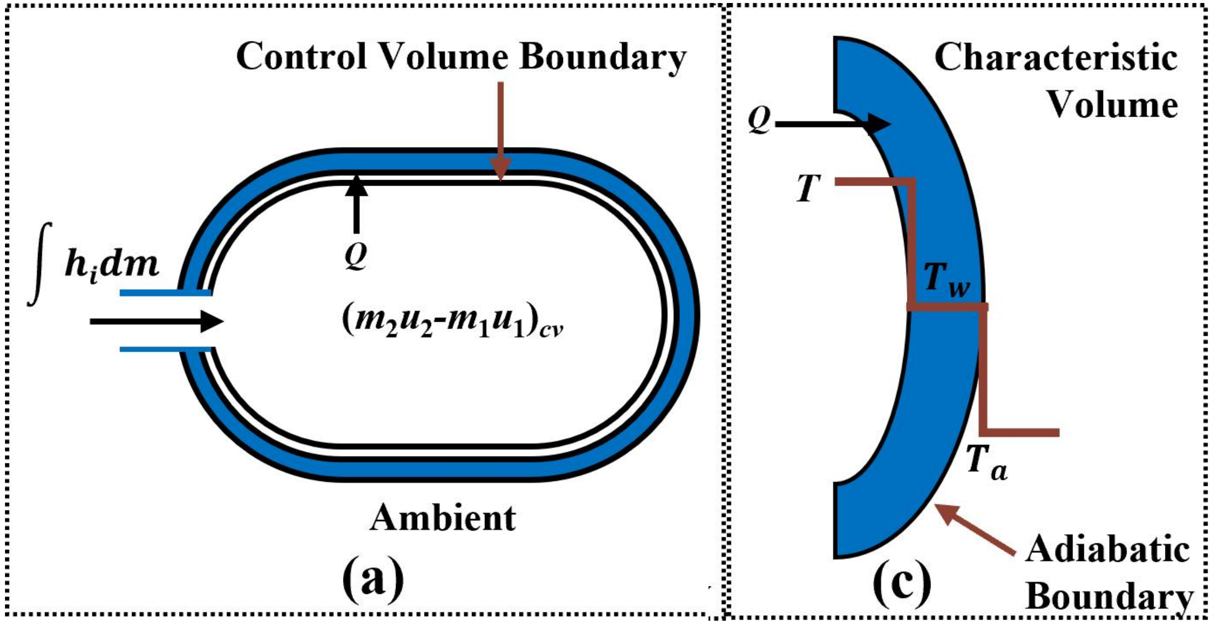
Heat transfer **energy balance**: Newton's Law of Cooling:

$$m_{\text{final}} c_v (T_{\text{adiabatic}} - \boldsymbol{T}_{\textbf{final}}) = \int_{t_{\text{initial}}}^{t_{\text{final}}} A_{\text{in}} a_{\text{in}} (T - T_w) dt$$

+

Approximation of integration:

$$\int_{t_{\text{initial}}}^{t_{\text{final}}} A_{\text{in}} a_{\text{in}} (T - T_w) dt = k_1 A_{\text{in}} a_{\text{ave}} \int_{t_{\text{initial}}}^{t_{\text{final}}} (T - T_w) dt = k_1 k_2 a_{\text{ave}} A_{\text{in}} t_{\text{final}} (T_{\text{final}} - T_{\text{wfinal}}) = K A_{\text{in}} t_{\text{final}} (\boldsymbol{T}_{\textbf{final}} - \boldsymbol{T}_{\textbf{wfinal}})$$



Improvements for MC method

Ending pressure determined by dual-zone dual-temperature model in modified MC method

The analytical solution for the final hydrogen temperature is obtained solving the above equation.

$$T_{\text{final}} = \frac{m_{\text{final}} c_v T_{\text{adiabatic}} + m_w c_w T_{\text{initial}}}{m_{\text{final}} c_v} - \frac{(m_w c_w)^2 T_{\text{initial}} (m_{\text{final}} c_v + \mathbf{K} A_{\text{in}} t_{\text{final}}) + \mathbf{K} m_{\text{final}} c_v T_{\text{adiabatic}} m_w c_w A_{\text{in}} t_{\text{final}}}{(m_{\text{final}} c_v)^2 m_w c_w + \mathbf{K} (m_{\text{final}} c_v)^2 A_{\text{in}} t_{\text{final}} + \mathbf{K} m_{\text{final}} c_v m_w c_w A_{\text{in}} t_{\text{final}}}$$

Correction term in modified MC method

$$\Downarrow$$

$$T_{\text{final}} = \frac{m_{\text{final}} c_v T_{\text{adiabatic}} + \mathbf{MC} T_{\text{initial}}}{\mathbf{MC} + m_{\text{final}} c_v}$$

Original MC method

Compare the analytical solutions of the final hydrogen temperature of the modified MC method and the original one:

In essence, the analytical solution of the final hydrogen temperature in the modified MC method **adds a correction term** due to the **distinction between hydrogen temperature and tank wall temperature**.

Improvements for MC method

Correction factors determined by simulation data from 0D1D model

- Calculate **capital *K*** from the above expressions.
- Substitute **average heat transfer coefficient** into capital *K* yields an equation for ***k*.**
- Use the **simulation data of the 0D1D model** fit the formula of ***k*.**
- A linear equation is obtained between ***k* and refuelling time**.
- Both the **slope D** and **intercept E** in the formula of *k* have a linear relationship with the **initial pressure**.

$$a_{\mathrm{ave}} = \bar{a}_{\mathrm{in}} = \frac{0.14\lambda\left(\frac{4}{\pi\mu}\right)^{0.67}\left(\frac{\bar{\dot{m}}}{d_{\mathrm{in}}}\right)^{0.67}}{D_{\mathrm{in}}}$$

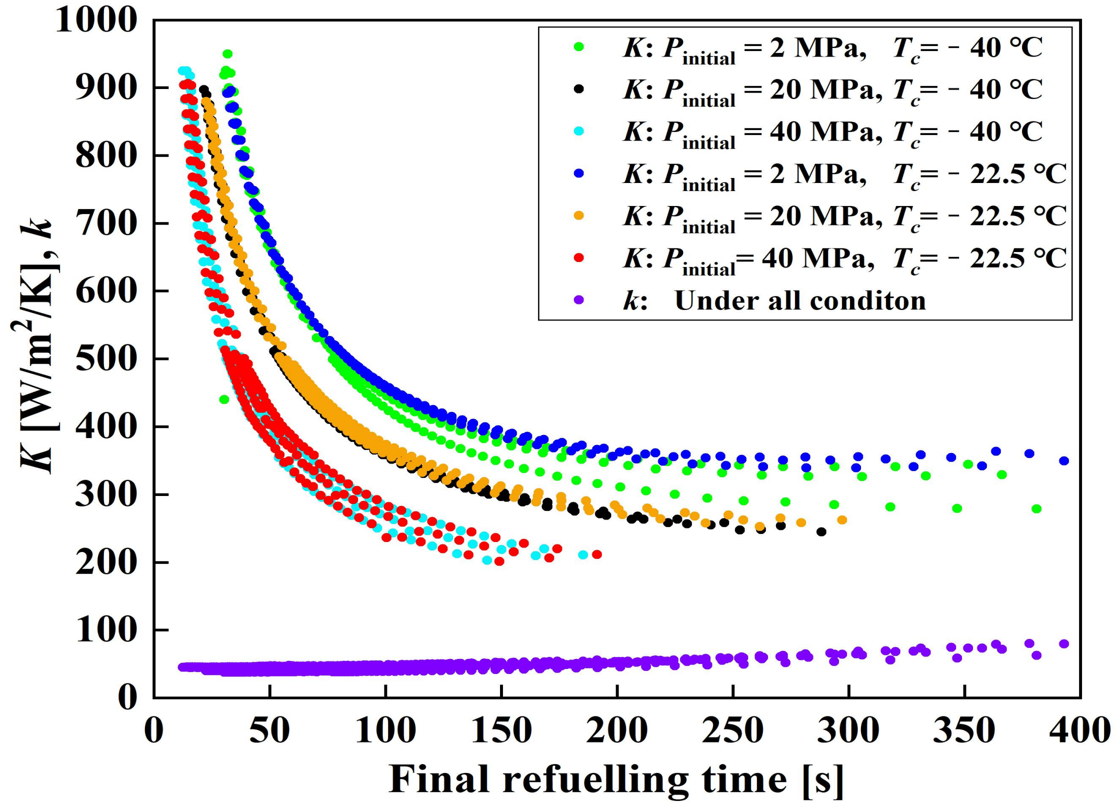
$$\boldsymbol{K} = k_1 k_2 \boldsymbol{a_{ave}} = \frac{m_{\mathrm{final}} c_v (T_{\mathrm{adiabatic}} - T_{\mathrm{final}})}{A_{\mathrm{in}} t_{\mathrm{final}} (T_{\mathrm{final}} - T_{w\mathrm{final}})}$$

$$\boldsymbol{k} = \frac{m_{\mathrm{final}} c_v (T_{\mathrm{adiabatic}} - T_{\mathrm{final}})}{A_{\mathrm{in}} t_{\mathrm{final}} (T_{\mathrm{final}} - T_{w\mathrm{final}}) \left(\left(\frac{\bar{\dot{m}}}{d_{\mathrm{in}}}\right)^{0.67} / D_{\mathrm{in}}\right)} = \frac{\boldsymbol{K}}{\left(\left(\frac{\bar{\dot{m}}}{d_{\mathrm{in}}}\right)^{0.67} / D_{\mathrm{in}}\right)}$$

$$\boldsymbol{k} = D t_{\mathrm{final}} + E$$

$$D = -0.0012 P_{\mathrm{initial}} + 0.1013 \ (\mathrm{R}^2=0.997)$$

$$E = 0.2982 P_{\mathrm{initial}} + 31.48 \ (\mathrm{R}^2=0.990)$$



Results and Discussion

Comparison for SOC results between the modified MC method and the original one

- The **modified final hydrogen temperature calculation method** is used instead of the original one to control the **ending pressure**. The control method of **refueling speed** still adopts that of **original MC method**. The simulations are conducted under a variety of initial and boundary conditions.
- Results show that the **final SOC** predicted by modified MC method is **more accurate** than that of the original one.

$$\boldsymbol{T}_{\mathbf{final}} = \frac{m_{\mathrm{final}} c_v T_{\mathrm{adiabatic}} + \mathbf{MC} T_{\mathrm{initial}}}{\mathbf{MC} + m_{\mathrm{final}} c_v}$$

$$\mathbf{MC} = \mathrm{AC} + \mathrm{BC} \ln \left(\frac{U_{\mathrm{adiabatic}}}{U_{\mathrm{initial}}} \right)^{1/2} + \mathrm{GC}\left(1 - e^{-\mathrm{KC}\Delta t}\right)^{\mathrm{JC}}$$

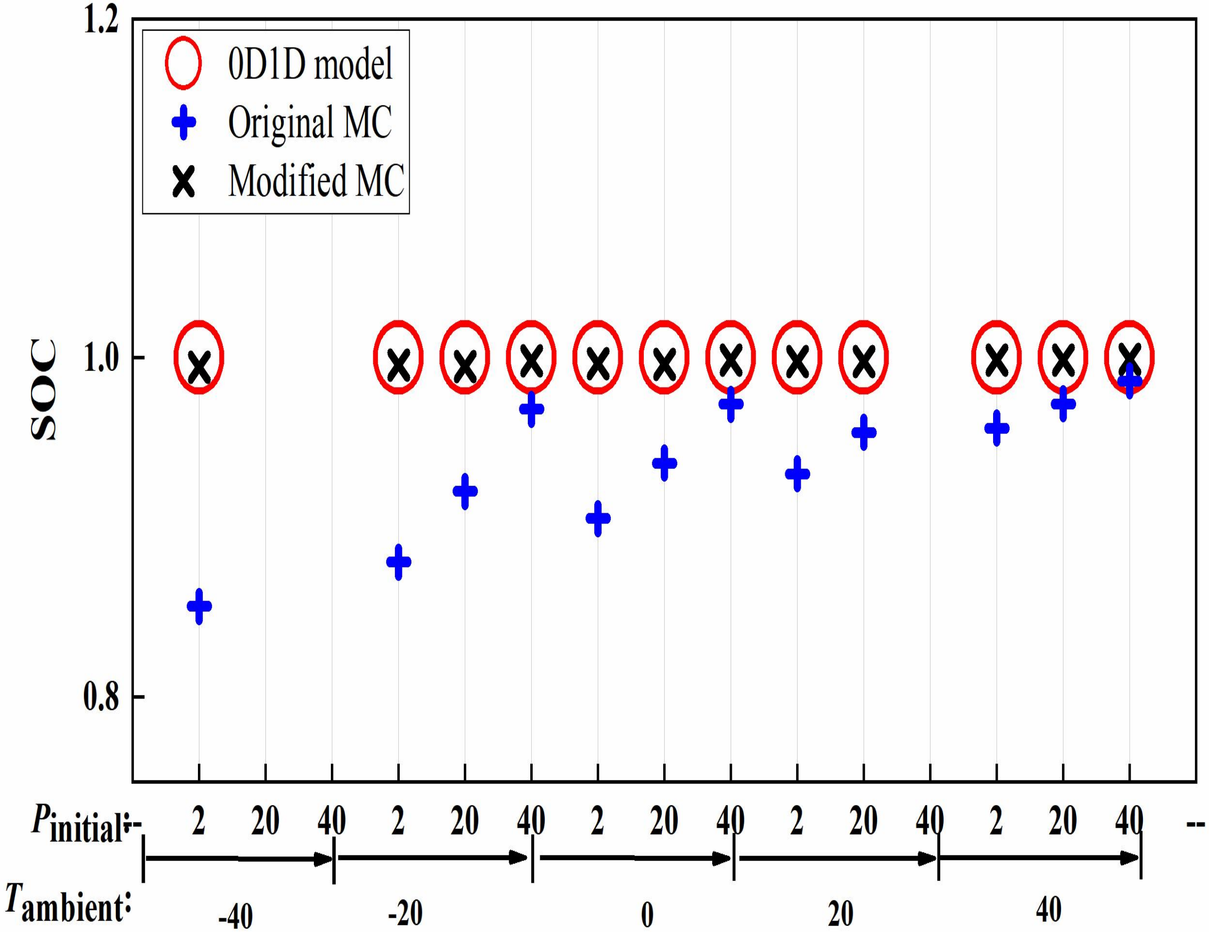
$$\boldsymbol{T}_{\mathbf{final}} = \frac{\boldsymbol{m}_{\mathbf{final}} \boldsymbol{c}_{\boldsymbol{v}} \boldsymbol{T}_{\mathbf{adiabatic}} + \boldsymbol{m}_{\boldsymbol{w}} \boldsymbol{c}_{\boldsymbol{w}} \boldsymbol{T}_{\mathbf{initial}}}{\boldsymbol{m}_{\mathbf{final}} \boldsymbol{c}_{\boldsymbol{v}}} - \frac{(\boldsymbol{m}_{\boldsymbol{w}} \boldsymbol{c}_{\boldsymbol{w}})^2 \boldsymbol{T}_{\mathbf{initial}} (\boldsymbol{m}_{\mathbf{final}} \boldsymbol{c}_{\boldsymbol{v}} + \boldsymbol{K} \boldsymbol{A}_{\mathbf{in}} \boldsymbol{t}_{\mathbf{final}}) + \boldsymbol{K} \boldsymbol{m}_{\mathbf{final}} \boldsymbol{c}_{\boldsymbol{v}} \boldsymbol{T}_{\mathbf{adiabatic}} \boldsymbol{m}_{\boldsymbol{w}} \boldsymbol{c}_{\boldsymbol{w}} \boldsymbol{A}_{\mathbf{in}} \boldsymbol{t}_{\mathbf{final}}}{(\boldsymbol{m}_{\mathbf{final}} \boldsymbol{c}_{\boldsymbol{v}})^2 \boldsymbol{m}_{\boldsymbol{w}} \boldsymbol{c}_{\boldsymbol{w}} + \boldsymbol{K} (\boldsymbol{m}_{\mathbf{final}} \boldsymbol{c}_{\boldsymbol{v}})^2 \boldsymbol{A}_{\mathbf{in}} \boldsymbol{t}_{\mathbf{final}} + \boldsymbol{K} \boldsymbol{m}_{\mathbf{final}} \boldsymbol{c}_{\boldsymbol{v}} \boldsymbol{m}_{\boldsymbol{w}} \boldsymbol{c}_{\boldsymbol{w}} \boldsymbol{A}_{\mathbf{in}} \boldsymbol{t}_{\mathbf{final}}}$$

$$\boldsymbol{k} = \frac{\boldsymbol{K}}{\left(\left(\frac{\bar{m}}{d_{\mathrm{in}}} \right)^{0.67} / D_{\mathrm{in}} \right)}$$

$$\boldsymbol{k} = \boldsymbol{D} t_{\mathrm{final}} + \boldsymbol{E}$$

$$\boldsymbol{D} = -0.0012 P_{\mathrm{initial}} + 0.1013 \ (\mathrm{R}^2 = 0.997)$$

$$\boldsymbol{E} = 0.2982 P_{\mathrm{initial}} + 31.48 \ (\mathrm{R}^2 = 0.990)$$



Conclusions

- For a complete hydrogen filling process, the **total amount of heat transferred by convection** between hydrogen and the inner wall of the storage tank can be expressed as an equation of the **final hydrogen temperature, final wall temperature, final refueling time, tank inner surface area and correction factor**.

- The correction factor k can be expressed as a **linear function with final filling time**. Both the **slope D** and **intercept E** in correction factor k have a linear function with **initial pressure.**

$\boldsymbol{k = Dt_{\text{final}} + E}$**, where** $\boldsymbol{D = -0.0012P_{\text{initial}} + 0.1013}$ **(R^2=0.997),** $\boldsymbol{E = 0.2982P_{\text{initial}} + 31.48}$ **(R^2=0.990)**.

- The **modified final hydrogen temperature** calculation method is used to replace the original one to control the **ending pressure**. The control method of **refueling speed** still adopts that of **original MC method**. Simulation results show that the **final SOC** predicted by modified MC method is **more accurate** than that of the original one.

- **Accurate estimation for final hydrogen temperature, ending pressure and final SOC is important** for improving hydrogen refuelling protocol and ensuring hydrogen refuelling **safety**.

Thanks for your attentions!

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