ESTIMATION OF FINAL HYDROGEN TEMPERATURE FROM REFUELING PARAMETERS

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For safety reasons, the final gas temperature in the hydrogen tank during refueling is limited to 85°C. Many experiments have been done for determining the final gas temperature in the hydrogen tank.

Lots of numerical simulations based on computational fluid dynamics have been performed and compared with experiments.

The rule of mixtures is a general weighted average method, which has been widely used to estimate various properties of a composite materials, porous media and multiphase system.

The effective (moderate) temperature of the mixture (cold and warm hydrogen, or hydrogen and tank wall, or even hydrogen and porous adsorbent) can be estimated based on the energy balance method.

We will apply the conception and the method to study effect of initial and final mass, effect of inlet and initial temperatures, effect of initial pressure and average pressure ramp rate (APRR), effect of initial pressure, ambient temperature and mass flow rate. The fittings agree very well with the original data.
Equations of Lumped Parameter Model

- **Mass balance equation**
  
  \[ \frac{dm}{dt} = \dot{m} \text{ where } \dot{m} = \dot{m}_{\text{in}} - \dot{m}_{\text{out}} \]

- **Energy balance equation**
  
  \[ \frac{d}{dt}(mu) = \dot{m}h + \dot{Q} \text{ where } \dot{m}h = \dot{m}_{\text{in}} h_{\text{in}} - \dot{m}_{\text{out}} h_{\text{out}} \]

\[ m = m_0 + \dot{m}t \]

\[ (m_0 + \dot{m}t) \frac{du}{dt} + mu = \dot{m}h + \dot{Q} \text{ where } \dot{Q} = a_f A_s (T_f - T) \]

\[ t^* = \frac{m_0}{\dot{m}} \quad q = \frac{\dot{Q}}{\dot{m}} \]

\[ (t^* + t) \frac{du}{dt} + u = h + q \]
Analytical Solution of Energy Equation

\[(t^* + t) \frac{du}{dt} + u = h + q \quad \text{where} \quad u = c_v T\]

\[h = c_p T_{\infty}\]

\[q = c_v \alpha (T_f - T)\]

\[\frac{dT}{dt} = (1 + \alpha) \frac{T^* - T}{t^* + t} \quad \text{where} \quad T^* = \frac{\gamma T_{\infty} + \alpha T_f}{1 + \alpha}\]

\[\alpha = a_f A_s / (c_v \dot{m})\]

\[\gamma = c_p / c_v\]

\[\frac{T^* - T}{T^* - T_0} = \left( \frac{1}{1 + \tau} \right)^{1+\alpha} \quad \text{where} \quad \tau = t / t^*\]
Weighted Averaging Form of Temperature

- Solutions of mass and energy equations
  \[ m = m_0 + \dot{m}t \quad \text{such that} \quad m/m_0 = 1 + \tau \]
  \[ t^* = m_0 / \dot{m}, \quad \tau = t / t^* \]

- Weighted averaging form of temperature
  \[ T = \mu' T_0 + (1 - \mu')T^* \quad \text{(Rule of mixture)} \]

\[ T^* - T \]
\[ T^* - T_0 \]
\[ \left( \frac{1}{1 + \tau} \right)^{1+\alpha} \]
\[ \mu = m_0 / m, \quad \mu' = \mu^{1+\alpha} \]
\[ \frac{T^* - T}{T^* - T_0} = \mu' \]
Analogy for Finial Gas Temperature

- Adiabatic tank not considering thermal capacity of the wall

\[ mc_v T = m_0 c_v T_0 + (m - m_0) c_p T_\infty \]

\[ T = \mu T_0 + (1 - \mu) T^* \quad \text{where} \quad T^* = \gamma T_\infty \]

- Adiabatic tank considering thermal capacity of the wall

\[ mc_v T + m_w c_w T_w = m_0 c_v T_0 + m_w c_w T_{w0} + (m - m_0) c_p T_\infty \]

If the conductive resistance of the tank wall is neglectable, the wall temperatures equal to the hydrogen temperatures, i.e.

\[ T_w = T \quad T_{w0} = T_0 \]

So \[ T = f_{MC} T_0 + (1 - f_{MC}) T^* \] (Rule of mixture)

where \[ f_{MC} = \frac{m_0 c_v + m_w c_w}{mc_v + m_w c_w} \]
Final / Initial Mass Ratio - Model

\[ T = \mu' T_0 + (1 - \mu') T^* \]

\[ \frac{T}{T_0} = \mu' + (1 - \mu') \frac{T^*}{T_0} \]

\[ \frac{T}{T_0} = A - (A - 1) \left( \frac{m}{m_0} \right)^{-C} \]

\[ \frac{T}{T_0} = \frac{T^*}{T_0} - \left( \frac{T^*}{T_0} - 1 \right) \mu' \]

\[ \mu' = \mu^{1+\alpha} = \left( \frac{m_0}{m} \right)^{1+\alpha} \]

\[ A = \frac{T^*}{T_0} \]

\[ C = 1 + \alpha \]

\[ \frac{T_{\text{mean}}}{T_i} = \left( A + B \left( \frac{m}{m_i} \right)^{1/2} \right)^C \]

RESULTS AND DISCUSSIONS

Final / Initial Mass Ratio - Results

\[
\frac{T}{T_0} = A - (A - 1) \left( \frac{m}{m_0} \right)^{-C}
\]

The derived two-parameter formula has the same ability to represent experimental data with the three-parameter formula.

\[
\frac{T_{\text{mean}}}{T_i} = (A + B \left( \frac{m}{m_i} \right)^{1/2})^C
\]

Inlet and Initial Temperatures - Model

\[ T = \mu' T_0 + (1 - \mu') T^* \]

\[ T^* = \frac{\gamma T_\infty + \alpha T_f}{1 + \alpha} \]

\[ T = \mu' T_0 + \frac{1 - \mu'}{1 + \alpha} \gamma T_\infty + \frac{1 - \mu'}{1 + \alpha} \alpha T_f \]

\[ \alpha = 0 \]

\[ T = \mu T_0 + (1 - \mu) \gamma T_\infty \]

Function of inlet and initial temperatures
RESULTS AND DISCUSSIONS

Inlet and Initial Temperatures - Results

\[ T = 0.59853T_0 + 0.60736T_{\infty} \]

Fitted parameter 0.60736 agrees with the number of 0.6 from linear curve fitting.

B. Acosta.
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\[ y = 0.6x + 35.4 \]
\[ R^2 = 0.9982 \]
Initial Pressure and APRR - Model

\[ T = \mu' T_0 + (1 - \mu') T^* \]

\[ T^* = \frac{\gamma T_0 + \alpha T_f}{1 + \alpha} = \frac{\gamma + \alpha}{1 + \alpha} T_f \]

\[ T_\infty = T_f \]

\[ T = \mu' T_0 + (1 - \mu') \frac{\gamma + \alpha}{1 + \alpha} T_f \]

\[ \alpha = \frac{B}{\dot{p}} = \frac{B}{APRR} \]

\[ \mu' \approx \mu = A p_0 \]

Function of initial pressure and APRR
The fitting based on the simulated data is better than that based on the experimental data because it has more data points.
Results and Discussions

Initial P, Ambient T and MFR - Model

\[ T = \mu' T_0 + \left(1 - \mu'\right)T^* \]

\[ T^* = \frac{\gamma T_\infty + \alpha T_f}{1 + \alpha} \]

\[ T = \mu' T_0 + \frac{1 - \mu'}{1 + \alpha} \gamma T_\infty + \frac{1 - \mu'}{1 + \alpha} \alpha T_f \]

\[ T_\infty = T_0, \quad T_f = T_0 \]

\[ T = \left(\frac{\gamma + \alpha}{1 + \alpha} - \frac{\gamma - 1}{1 + \alpha} \mu'\right)T_0 \]

\[ T = \left(\mu' + \frac{1 - \mu'}{1 + \alpha} \gamma\right)T_0 + \frac{1 - \mu'}{1 + \alpha} \alpha T_f \]

Negatively linear with initial pressure

Positively linear with ambient temperature

\[ T_0 = 293.15K \]

\[ \gamma = 1.4 \]

\[ \mu' = K_p p_0 \]

\[ \alpha = K_m / \dot{m} \]
Effects of (a) initial pressure, (b) ambient temperature, (c) hydrogen mass flow rate on final hydrogen temperature compared with data.

Conclusion

- The energy, like density and heat capacity, is not sensitive with the structure of the mixture or composites. Therefore, the upper bound of the rule of mixtures is used to estimate the hydrogen temperature.
- The analytical solution of hydrogen temperature behaves in an analogous way as the rule of mixtures. The final hydrogen temperature is the weighted average of initial temperature and a characteristic temperature which is related the inflow enthalpy of hydrogen. The weighted factor is initial heat capacity fraction.
- The simple uniform formula, inspired by the concept of the rule of mixtures with its weighted factors obtained from the analytical solution of thermodynamic model, is applied to fit published experimental or simulated results.
- These results show effect of initial and final mass, effect of inlet and initial temperatures, effect of initial pressure and average pressure ramp rate (APRR), effect of initial pressure, ambient temperature and mass flow rate. The fittings agree very well with the original data.
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