INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 41 (2016) 6610–6617

Available online at www.sciencedirect.com

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journal homepage: www.elsevier.com/locate/he

Standardized equation for hydrogen gas compressibility factor for fuel consumption applications

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ARTICLE INFO

Article history:
Received 4 October 2015
Received in revised form
25 February 2016
Accepted 1 March 2016
Available online 24 March 2016

Keywords:
Equation of state
Hydrogen gas compressibility factor
Fuel consumption
Polynomial fitting

ABSTRACT

The hydrogen gas compressibility factor is a key parameter when the pressure–temperature method is used to measure hydrogen fuel consumption. Based on the data from the National Institute of Standards and Technology (NIST) Chemistry WebBooks, a standardized equation for hydrogen gas compressibility factor based on pressure and temperature dependent terms is developed by means of polynomial fitting. The equation agrees with the NIST density data to within 0.01% from 220 K to 500 K with pressures from 0.1 MPa to 100 MPa, and to within 0.003% from 270 K to 500 K with pressures from 10 MPa to 100 MPa, which has higher accuracy compared with the Lemmon equation. Experimental research shows that the hydrogen consumptions calculated by using the proposed equation are in good consistency with the results measured by the flowmeter. The proposed equation can be easily used in the calculation of hydrogen fuel consumption.

Introduction

The escalating energy crisis and increasingly serious environmental pollution have driven the need for new and environment-friendly fuels in the auto-industry. Hydrogen fuel cell vehicle is recognized as an effective way of hydrogen energy utilization and reduction of environmental pollution. Along with the rapid development of hydrogen fuel cell vehicle, an accurate measurement method of gaseous hydrogen fuel consumption becomes a necessity.

The Society of Automotive Engineers standard SAE J2572 *Recommended Practice For Measuring Fuel Consumption And Range Of Fuel Cell And Hybrid Fuel Cell Vehicles Fueled By Compressed Gaseous Hydrogen* and the proposed Chinese national standard draft *Fuel cell hybrid electric vehicles Energy consumption Test*

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http://dx.doi.org/10.1016/j.ijhydene.2016.03.004

methods both approve three methods to measure hydrogen fuel consumption, which are gravimetric method, fuel flowmeter method, and pressure–temperature method. Compared with the other two methods, the pressure–temperature method is simple and has better repeatability. It only needs the determination of the equilibrium temperature and pressure of hydrogen gas before and after usage within a storage tank of known and essentially fixed volume, and use the corresponding compressibility factor (or density) to calculate gaseous hydrogen fuel consumption. The key to make the method convenient and efficient is to quickly and accurately obtain gaseous hydrogen compressibility factor at different temperatures and pressures.

At present, there are three ways to get the compressibility factor: query the NIST Chemistry WebBooks [1], query a compressibility factor graph, or calculate the compressibility factor by equations of state. SAE J2572 standard approves the way to query the NIST Chemistry WebBooks. This method and the method of querying a compressibility factor graph are inconvenient, and the latter is more prone to error. Some scholars studied equations of state for hydrogen gas based on density and temperature dependent terms [2–9]. However, this form is inconvenient to use in the fuel consumption application since these equations must be solved in an iterative manner in order to provide the density in terms of pressure and temperature.

Chen [10], Lemmon [11,12], Davarnejad [6] obtained hydrogen compressibility factor equations based on pressure and temperature dependent terms. Chen's equation is very simple, but its error is large. Davarnejad's equation has lots of coefficients, and its calculation results compared with its fitting data are quite accurate, but in the pressure above 10 MPa, its error with NIST data is also large, restricting its widespread usage. The relative error of these two equations with the standard hydrogen density data from the NIST are unable to be controlled within 0.01%, even more than 3%, thus fail to meet the general requirement that the calculation accuracy of equations be controlled within 0.01% compared with the NIST data. Lemmon equation [12] has the highest accuracy in comparison with other hydrogen compressibility factor equations based on pressure and temperature dependent terms. However, from 220 K to 255 K with pressures from 70 MPa to 90 MPa, the density error of Lemmon equation relative to the NIST data is not limited within 0.01%.

As onboard hydrogen storage pressure increased, the filling pressure now is at most up to 87.5 MPa. Using the MATLAB software, this paper develops a more accurate hydrogen compressibility factor equation to meet the general requirement in high pressure range (from 0.1 MPa to 100 MPa).

Equation for gaseous hydrogen compressibility factor

Pressure and temperature scope

In terms of pressure, to improve driving range, the nominal working pressure of high-pressure hydrogen storage tank of hydrogen fuel cell vehicles is usually 70 MPa, with filling pressures at most up to 125% of the nominal working pressure, namely 87.5 MPa.

In terms of temperature, the temperature of onboard hydrogen storage tank and pressure vessels in hydrogen refueling station is under the influence of the surrounding temperature, and affected by the filling rate in the filling process. The current statistics show that the temperature of north latitude 45°area will happen −40 °C of extreme weather, low latitudes would happen extremely high temperature of 50 °C. And in the process of fast filling, the temperature of hydrogen gas in cylinders will rise, in order to avoid too high temperature which may lead to the degradation of cylinder materials, UN GTR 13 *the hydrogen fuel cell vehicles global technical regulations* [13] allows the hydrogen in the process of fast filling to reach a highest temperature of 85 °C. So the working temperature range for onboard high pressure hydrogen storage tanks is determined between −40 °C and 85 °C.

Thus, the pressure scope is set between 0.1 MPa–100 MPa, including 0.1 MPa–87.5 MPa, and the temperature range is set between 220 K–500 K, including 233.15 K–358.15 K, namely −40 °C to 85 °C.

Fitting data

The data fitted in this paper are provided by thermodynamic properties database of the National Institute of Standards and Technology. It is calculated by REFPROP 8.0, a software developed by the NIST to calculate the thermodynamic property. REFPROP 8.0 adopts the currently available most accurate calculation model for thermodynamic property data of fluids, such as H_2, N_2, CO_2, and mixed gas in a certain proportion. For hydrogen, REFPROP 8.0 adopts the Leachman equation to calculate the thermodynamic property, which has the smallest uncertainty [9]. The Leachman equation is a 14-term Helmholtz energy equation, based on temperature and density dependent terms, with uncertainty of 0.1% from 220 K to 250 K with pressures up to 40 MPa, and 0.04% from 250 K to 450 K with pressures up to 300 MPa. Therefore, the equation developed from the NIST data (in other words developed from the Leachman equation) with high fitting precision can ensure its calculation uncertainty minimal.

Fitting method

The equation fitted in this paper, as shown in Eq. (1), is an expression for hydrogen compressibility factor as a function of pressure and temperature. To be able to obtain the equation by a simple polynomial fitting method, and conveniently control the calculation precision of fitting equation, the values of the exponents on pressure and temperature are set as integers. Eq. (2) is used to calculate the gaseous hydrogen density based on the results of Eq. (1).

$$Z = \sum_{i=1}^{6}\sum_{j=1}^{4} v_{ij} p^{i-1} (100/T)^{j-1} \quad (1)$$

$$\rho = Mp/(ZRT) \quad (2)$$

where v_{ij} is the coefficients, p is the pressure, MPa, T is the absolute temperature, K, ρ is the density, kg/m^3, M is the molar