Short Calculation of Particle Transport Properties in Hydrogen Gas

Byung Uk Lee[*]

Aerosol and Bioengineering Laboratory, Department of Mechanical Engineering, College of Engineering, Konkuk University, 1 Hwayang-dong, Gwangjin-gu, Seoul, 143-701, Korea

ABSTRACT

Usage of hydrogen gas has increased due to fast development of the fuel cell technology. Currently, little attention is paid to particles in hydrogen gas, however, particles in hydrogen gas have great potential to affect hydrogen equipments. Here, a short calculation of particle transport properties in hydrogen gas is conducted via comparison with aerosol properties.

Keywords: Hydrogen; Transport property; Diffusion; Thermophoresis; Migration.

INTRODUCTION

Hydrogen gas has received renewed attention recently for its potential as a global fuel source, since there is growing interest in hydrogen fuel cells which may replace the ubiquitous usage of hydrocarbon fuel sources (Moran and Shapiro, 2004; Hirschenhofer *et al.*, 1998). In the hydrogen gas systems, it has been found that particles were generated in several processes. For examples, carbon aggregates were generated during the reforming process of methane gas during hydrogen gas generation process (Horng *et al.*, 2006), metal particles were generated in hydrogen transport pipes due to the embrittlement reaction between hydrogen gas and the metal surfaces (Norbeck *et al.*, 1996), and impurity particles were generated in the hydrogen hybrid combustion engines (Das, 1991). Also, it was found that carbon particles were generated in the hydrogen fuel cells due to the deposition of carbon during the adsorption of CO and CO_2 gases, which were impurity gases, onto the metal bodies (Sone *et al.*, 2000). These particles, which are generated by various mechanisms in hydrogen gas, can decrease the efficiency of hydrogen gas transport by the plugging of the gas channels and they may induce some operational degradation in the hydrogen fuel cell plants. Also, it was suspected that particles in hydrogen gas might cause malfunction on hydrogen gas sensors (Mor *et al.*, 2004). As the usage of hydrogen gas grows, it is necessary to study properties and control methodologies for particles or solid impurities in hydrogen gas, in order to operate or improve the systems of hydrogen gas efficiently.

Particle transport properties in hydrogen gas would differ from those of airborne particles, aerosols, due to a significant difference between the properties of air and those of hydrogen gas. Transport properties of aerosols have been thoroughly studied (Hinds, 1999; Willeke and Baron, 1993; Friedlander, 2000); however, few studies have been conducted regarding the properties of particles in hydrogen gas. In this study, several brief estimations for particle transport properties (Friedlander, 2000) in hydrogen gas were conducted, and the values of properties were compared with aerosol properties. The operation temperatures of fuel cells and hydrogen gas transport depend on the fuel cell types. For example, a phosphoric acid fuel cell and a molten carbonate fuel cell are operated at 450 K and 920 K, respectively. In this study, the operation temperature of a polymer electrolyte membrane fuel cell was selected because it had the highest power density of all the fuel cell classes and good start-stop capabilities. Also, low temperature operation (less than 360 K) makes the polymer electrolyte membrane fuel cell suitable for portable applications (O'hayre *et al.*, 2009). Therefore, we chose 300 K and 350 K for calculation of the particle transport properties; however, it is not so difficult to estimate the properties under other temperature conditions using our suggested methods with the gas properties data under specified temperature conditions.

DIFFUSION, THERMOPHORESIS, AND MIGRATION VELOCITIES

Gas Properties

All differences in transport properties of particles come from the difference of gas properties of air and hydrogen gas. Gas properties of air (mostly nitrogen and oxygen) and hydrogen are listed in Table 1 at 300K and atmospheric pressure (1 atm). Hydrogen gas has a density around 14 times lighter and a viscosity 2 times smaller compared with

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[*] Corresponding author. Tel.: +82-2-450-4091;
  Fax: +82-2-447-5886
  E-mail address: leebu@konkuk.ac.kr

Table 1. Gas properties of air and hydrogen at 300K and atmospheric pressure (1atm) (Incropera and DeWitt, 1990).

Properties	Air	Hydrogen (H_2)
Density (ρ)	1.1614 kg/m^3	0.0808 kg/m^3
Absolute viscosity (μ)	184 × 10^{-7} Ns/m^2	89.6× 10^{-7} Ns/m^2
Thermal conductivity (k)	26.3 × 10^{-3} W/m K	183 × 10^{-3} W/m K
Specific heat (Cp)	1.007 kJ/kg K	14.31 kJ/kg K

air. In addition, hydrogen gas has a thermal conductivity around 7 times higher and a specific heat value 14 times larger than air. The significant differences between such basic gas properties can cause differences in the characteristics of gas movement as well as particle transport properties. The representative example for the difference of gas movement is the Reynolds number. The Reynolds number, which has been regarded as a key parameter to analyze fluid flow and a guideline for judging laminar flow and turbulent flow (Fox and McDonald, 1994), is shown in the following formula (1):

$$Re = \frac{\rho V d}{\mu} \tag{1}$$

where ρ is the fluid density, V is the flow velocity, d is the characteristic length, and μ is the absolute viscosity. When using the same geometry (d) and flow velocity (V), the Reynolds number of hydrogen gas system is 7 times smaller than the value of air at 300 K and atmospheric pressure. Therefore, we expect a more laminar flow of hydrogen gas than air.

Transport Properties - Diffusion Coefficient

The ratios of the major transport properties of particles in hydrogen and aerosols are shown in Tables 2 and 3. The ratios of the transport properties were calculated with respective assumptions which are introduced in the following sections. The ratios were calculated at 300K (normal temperature) and 350K (relatively hot condition) in Table 2.

The diffusion coefficient is shown in the following formula (Hinds, 1999; Friedlander, 2000):

$$D = \frac{kTC_c}{3\pi\mu d_p} \tag{2}$$

where, k is Boltzmann's constant, T is temperature, C_c is the slip correction factor, and d_p is the particle diameter. Assuming conditions of the same temperature, the same particle diameter, and the same slip correction factor, the diffusion coefficient of particles in hydrogen gas is estimated to be twice larger than the value in air due to the difference of viscosity. Therefore, the diffusion effect of particles is expected to be much more significant in hydrogen gas compared with that in air. For example, filters for particles in hydrogen gas should be designed in considering this different diffusion coefficient.

Transport Properties - Thermophoresis

Several formulas have been suggested to describe thermophoresis (Chang *et al.*, 1995; Hinds, 1999; Lee and Kim, 2001). Most of them have the following form:

$$V_{th} = -F\frac{\mu\nabla T}{\rho_g T} \tag{3}$$

where F is the factor that depends most on particle properties, μ is the absolute viscosity, T is the temperature, and ρ_g is the fluid density. Assuming conditions where F and the

Table 2. Ratios of transport properties of particles in hydrogen and aerosols at 1 atm under the assumption of the same particle diameter and the same slip correction factor.

Transport properties	$\dfrac{\text{Property in hydrogen gas}}{\text{Property in air, aerosols}}$ at 300 K	$\dfrac{\text{Property in hydrogen gas}}{\text{Property in air, aerosols}}$ at 350 K
Diffusion coefficient	2.05	2.11
Thermophoretic velocity	7.00	6.82
Migration velocity	2.05	2.11

Table 3. Ratios of transport properties of particles in hydrogen and aerosols with varying particle size at 1 atm and 300 K (*under the assumption of constant F and the constant temperature gradient in thermophoresis calculation).

Transport properties	$\dfrac{\text{Property in hydrogen gas}}{\text{Property in air, aerosols}}$ 10 µm	$\dfrac{\text{Property in hydrogen gas}}{\text{Property in air, aerosols}}$ 1 µm	$\dfrac{\text{Property in hydrogen gas}}{\text{Property in air, aerosols}}$ 0.1 µm
Diffusion coefficient	2.08	2.30	3.36
Thermophoretic velocity*	7.00	7.00	7.00
Migration velocity	2.08	2.30	3.36

temperature gradient are same, the thermophoretic velocity will increase 7 times higher in hydrogen gas compared with that in air due to the difference of viscosity and density. Therefore, the particle movement is estimated to be much more sensitive to temperature gradient in hydrogen gas.

Transport Properties - Migration Velocities

Generally, the migration velocities of particles due to specific forces can be calculated by the following equation:

$$Force = \frac{3\pi\mu V_{mig} d_p}{C_c} \qquad (4)$$

where V_{mig} is the migration velocity due to some specific force, such as electric force. If the force and other particle properties are same, the migration velocities of particles will be two times larger in hydrogen gas than in air due to the decrease of the absolute viscosity. Therefore, external forces can be more effective to control particles in hydrogen gas compared with aerosols.

Additionally, the Stokes number, which is a key parameter associated with particle inertia and impaction in the flow (Friedlander, 2000), will be twice larger in hydrogen gas than its value in air under the condition of same properties of particles. Therefore, particles in hydrogen gas can be affected more by their inertia compared with aerosols.

Consideration of particle size

The transport properties also depend on the types of flow regime, which are continuum, free molecular, and intermediate flows. The classification of flow regimes is decided by the following Knudsen number:

$$Kn = \frac{2\lambda}{d_p} \qquad (5)$$

where λ is the gas molecular mean free path, which is one of the gas properties, and d_p the particle diameter. A $Kn \ll 1$ indicates a continuum flow regime and $Kn \gg 1$ indicates a free molecular flow regime. The intermediate Kn range is approximately 0.4–20 (Willeke and Baron, 1993). The values of the mean free path of air and hydrogen are 0.0665 μm and 0.123 μm, respectively, under normal temperature and pressure conditions of 20°C and 1 atm (Rader, 1990). Therefore, the border lines between the free molecular, intermediate, and continuum regimes are around d_p = 6.6 nm and 0.3 μm for particles in air; and around d_p = 12 nm and 0.6 μm for particles in hydrogen gas, with Kn = 20 and Kn = 0.4, respectively.

This calculation means that, if particles in hydrogen gas are larger than 0.6 μm, then it is possible to use the continuum assumption without significant errors; this particle size is twice as large as that in air. The particle size spectrum for the free molecular regime is broader in hydrogen gas (up to 12 nm) than aerosol particles (up to 6.6 nm). Therefore, the analysis implies the particles in hydrogen gas are more likely to be influenced by free molecular effects than aerosol particles. Table 3 shows the estimation of the ratios

of the major transport properties of particles in hydrogen and aerosols with varying particle size.

BRIEF SUMMARY

Overall, particle transport properties in hydrogen gas, which have rarely been considered, were estimated in this study by using several dimensional calculations. The accuracy of the calculation and analysis presented in this study is limited by the accuracy of the gas data from the cited references, which varied from data to data according to their total counts of significant digits. It is estimated that particle transport properties in hydrogen gas can be significantly different from aerosol properties. These differences should be considered in studying and developing control equipments for particles in hydrogen gas.

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