

Developing Method Using CFD to Design Hydrogen Isolation Structure with Waterproof and Dustproof Filters

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ABSTRACT

With a view to still greater compactness and lighter weight in fuel cell systems, a method using computational fluid dynamics was developed to obtain the filter properties necessary to design a hydrogen isolation structure with waterproof and dustproof filters. The filter properties were identified by measuring gas pressure and concentration on both sides of the filter and then using computational fluid dynamics to simulate the measurements to reproduce their content.

The identified properties were confirmed to be versatile and applicable for other initial conditions of gas type, flow, and concentration.

The design method was also validated by comparing the gas concentrations obtained from measurement by a simple testing apparatus to the results of computational fluid dynamics using identified properties. It was confirmed that satisfactory prediction was possible even under conditions of extremely low gas flow.

As a result, a design method using computational fluid dynamics was developed to realize a safer, more compact, and lighter-weight hydrogen isolation structure with filters.

1. Introduction

In order to enlarge the interior space of the Honda CLARITY FUEL CELL, the fuel cell powertrain was installed under the front hood⁽¹⁾ and hydrogen (H₂) related parts were enclosed in the hydrogen isolation structure shown in Fig. 1, thereby realizing hydrogen safety. The hydrogen isolation structure was made up of three elements: a barrier, hydrogen sensors, and ducts. If the hydrogen-related parts were damaged due to a vehicle collision or other such reason, then hydrogen could leak inside the isolation structure. That leakage would be detected by the hydrogen sensors and the supply of hydrogen would be shut off.

The hydrogen is discharged outside the vehicle through the ducts to reduce its concentration below the flammable threshold, thereby helping ensure the safety of the vehicle.

Even during normal operation, an extremely low flow of around several cm³/min of hydrogen can pass from the stack through the stack sealing material and permeate

the hydrogen isolation structure. This happens because hydrogen molecules are very small. When this hydrogen exceeds the sensor's threshold concentration value for detection of irregularities, then the system will determine that hydrogen leakage has occurred and will shut down even in normal operation. Therefore, the hydrogen isolation structure needs to discharge that minute amount of hydrogen so as not to exceed the sensor threshold. Consequently, computational fluid dynamics (CFD) was employed to confirm for design reasons that the hydrogen concentration would remain below the threshold even if hydrogen permeation were to occur.

Hydrogen safety requirements have to be met, after which it is desirable for the hydrogen isolation structure to be made more compact and lighter in weight. This can be expected to be achieved by attaching multiple waterproof and dustproof filters in place of the ducts to discharge hydrogen. This report will describe the creation of the CFD method for designing the hydrogen isolation structure with filters and the validity of the method.

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2. Development Goals

Figure 2 shows a conceptual diagram of the hydrogen isolation structure with filters. Air-permeable waterproof and dustproof filters are placed in part of the barrier, and hydrogen that is below the flammable threshold is discharged through the filters into the space under the front hood. In this way, the ducts are discontinued and the isolation structure can be made more compact and lighter in weight. The amount of hydrogen discharged through the filters is determined by the following three factors.

- (1) Installed location: Hydrogen is lighter than air, so it accumulates in the upper interior of the isolation structure. Therefore the amount of hydrogen discharged varies according to the installed locations of the filters.
- (2) Area: The greater the area, the more hydrogen will be discharged.
- (3) Material properties: The permeability of the material itself will change the amount of hydrogen that is discharged.

Since the hydrogen permeation amount varies according to the vehicle driving circumstances and ambient

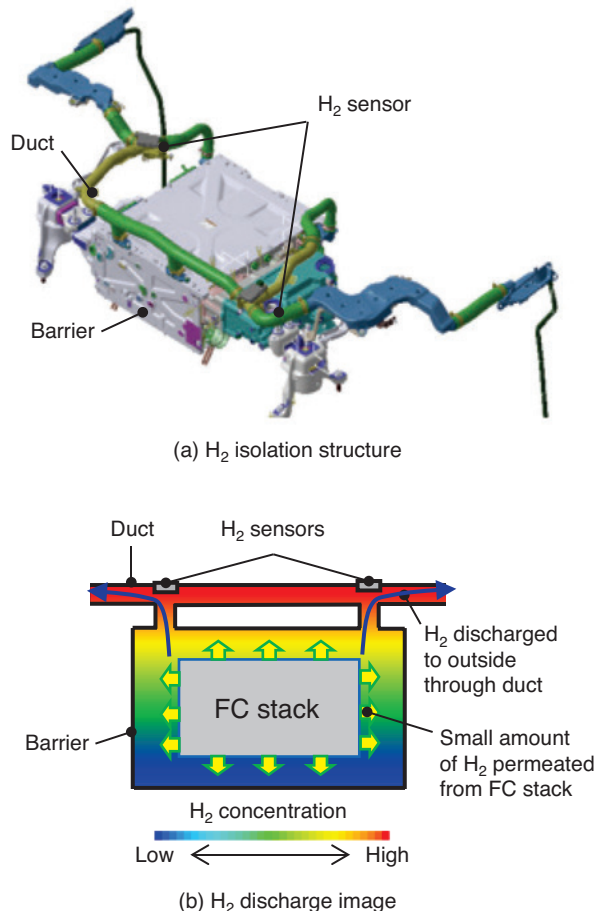


Fig. 1 H₂ isolation structure in Honda CLARITY FUEL CELL

temperature, the properties used for CFD are required to be flexibly applicable under a variety of initial conditions.

When designing with CFD, a three-dimensional model of the inside and outside of the hydrogen isolation structure with filter space that reproduces its location and area should be made first. Next, the filter properties are defined, then the concentration of hydrogen is calculated relative to the amount of hydrogen as initial condition. Then the area and location of the filters as well as the shape of the hydrogen isolation structure are decided to achieve the hydrogen concentration inside it that keeps below the threshold. Therefore, the filter properties should be obtained before CFD.

However, using dustproof and waterproof filters for hydrogen ventilation is not normal usage, so that the phenomenon of low-flow of hydrogen permeating filters is not generally envisioned. Consequently, the properties needed for the present design do not exist and a method for obtaining them has not been established.

For this research, therefore, a new method for obtaining the properties was to be created and a low-flow gas CFD method was to be established.

The aims of this research are defined as follows:

- (1) To establish a method for obtaining the properties for extremely low-flow gas that permeates filters that are provided as input to CFD, and to obtain the values
- (2) To be versatile and usable under different permeation amount and temperature conditions
- (3) To have the CFD predicted values be a quantitative match with measured values

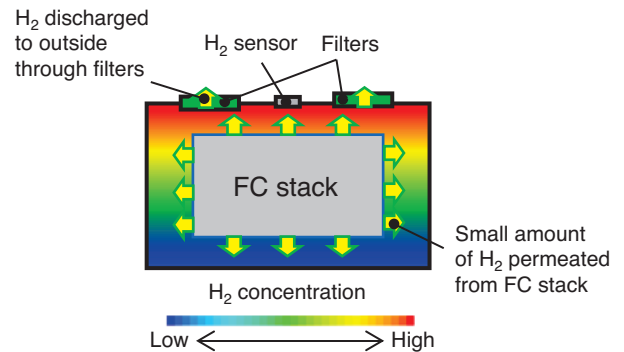


Fig. 2 H₂ discharge image of H₂ isolation structure with filters

3. Creating a Method for Obtaining Extremely Low-flow Gas Properties Through Filters

3.1. Fundamental Equations

The fundamental equations expressing the correlation between the various parameters and the phenomenon of gas transport are shown below. Equation (1) is the advection equation (the Darcy equation), and Eq. (2) is the diffusion equation.

$$\frac{dP}{dx} = -A_1 \mu v + A_2 \frac{1}{2} \rho v^2 \quad (1)$$

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (2)$$

A_1 : Coefficient of viscous resistance [$1/m^2$]

A_2 : Coefficient of inertial resistance [$1/m$]

C : Gas concentration [mol/mol]

D : Diffusion coefficient [m^2/s]

P : Pressure [Pa]

t : Time [s]

v : Gas flow velocity [m/s]

x : Distance [m]

ρ : Mixed gas density [kg/m^3]

μ : Mixed gas viscosity [$Pa \cdot s$]

Here the filter properties are A_1 , A_2 , and D . These three properties are determined from the pressure gradient (advection) and the concentration gradient (diffusion) shown in Eqs. (1) and (2). The filter properties can be expressed by advection and diffusion just as in a regular flow field.

The influence of advection is expressed by an equation correlating pressure and flow velocity, and it is typically shown in a quadratic function. The coefficients of that quadratic function are the coefficient of viscous resistance A_1 and the coefficient of inertial resistance A_2 .

The influence of diffusion, as shown in the diffusion equation, arises from the concentration difference. In a medium or larger flow field, advection dominates this flow field with large v on the right side of Eq. (1). Influence of advection decreases and the influence of diffusion increases in a low flow field. Therefore it becomes important to clarify the value of D in distinction to A_1 and A_2 in a minute flow field. For that purpose, a measuring apparatus was devised and measurements of A_1 and A_2 were made.

3.2. Pressure and Concentration Measuring Apparatus and Measurement Method

To isolate the values of A_1 , A_2 , and D , a filter was installed between two spaces and a measuring apparatus was created with the capability to obtain time series data on pressure and concentration simultaneously on both sides. A method was further devised to reproduce the measurements by CFD and obtain the CFD parameters that are needed to develop the design.

Figure 3 shows the measuring apparatus that makes pressure and concentration measurements on both sides of the filter. A straight channel of 20-mm inner diameter was made the flow path. To obtain the properties of the mixture gas, gas inlets are placed on the left and right. Two different types of gas, Gas A and Gas B, are sealed into the flow channel with a closed valve separating them. Then steps are taken to simultaneously supply Gas A, close the Gas A outlet and the Gas B inlet, and open the valve. This creates

a unidirectional flow from the A side to the B side through the filter and all the gas is discharged to the Gas B outlet.

The filters are fixed with aluminum plates as shown in Fig. 4. Both types of filter, sheet filter shown in (a) and button filter shown in (b) can be attached. The diameter of the mounting hole of the filter was 10 mm so as not to distribute horizontally to the filter surface. The plates with filters assembled are sealed between flanges with O-rings on both sides. Concentration sensors and pressure sensors are installed and measurements are made on both sides of the filter. When making measurements, the room temperature and inlet Gas A temperature should be the same so as not to incur measurement error due to the temperature difference.

Concentration sensors (C_2 and C_3) and pressure sensors (P_2 and P_3) are both located on both sides of the filter. Time series measurements were made starting immediately after the valve was opened and until all sensor values reached a steady state.

At this time, the relationship between the pressure drop $P_2 - P_3$ measured under multiple gas flow conditions and the gas flow velocity, which was gas flow divided by cross-sectional area, is expressed in the form of the quadratic function shown in Eq. (3) and Fig. 5. At this time, a and b are coefficients.

$$\frac{P_2 - P_3}{x} = av + bv^2 \quad (3)$$

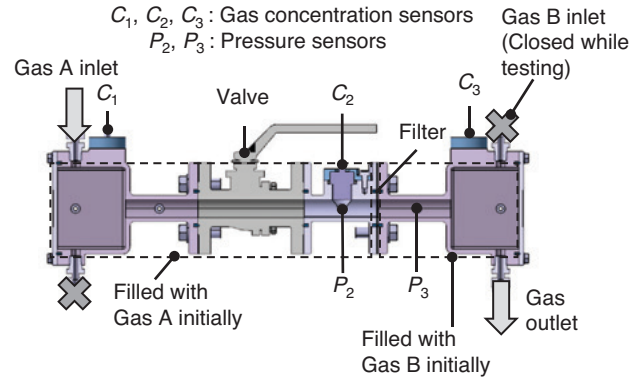


Fig. 3 Filter pressure drop and gas concentration measuring apparatus

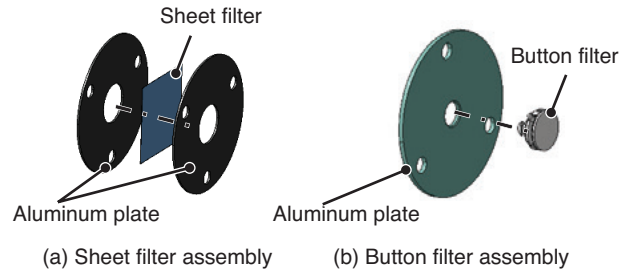


Fig. 4 Filter assembly

Since Eq. (3) is identical to Eq. (1), it follows that these relational expressions apply:

$$-A_1\mu = a \quad (4)$$

$$A_2 \frac{1}{2} \rho = b \quad (5)$$

From these, A_1 and A_2 can be derived.

3.3. Identification of Diffusion Coefficient D by CFD Analysis

Concentrations on both sides of the filter are not subject to difference like pressure, but the same value. C_2 and C_3 approach the same value over time. For this reason, a different method is needed to obtain D .

Therefore, the measurement above was reproduced in CFD to identify D that could obtain the same time series of C_2 and C_3 . A mesh model of the space inside the measuring apparatus and the filter shown in Fig. 3 was created. The Gas A space was filled with Gas A and Gas B space was filled with Gas B as the initial condition. From that state, Gas A was introduced at the specified flow and concentration, and transient calculations were performed to simulate the Gas A flow to the Gas B outlet through the filter (Fig. 6).

By assigning the values of A_1 , A_2 , and D to the filter portion of the CFD, the kinds of phenomena measured in testing are also expressed in CFD. That is, the pressure difference between P_2 and P_3 and the C_3 concentration rise delay due to the filter inhibiting the gas transport (Fig. 7). This delay varies according to A_1 , A_2 , and D . Because A_1

and A_2 are identified from measurement, the remaining D is identified by CFD. This method can be applicable even under low-flow gas conditions because a larger difference between C_2 and C_3 can be obtained under the conditions.

In identifying D , multiple CFD results with different values of D are needed, as in Fig. 8. The square of the difference between measured values and CFD values in C_2 and C_3 was calculated every second and each Δ_{sum}^2 was obtained to integrate them by the specified time t_e . Δ_{sum}^2 is as shown in Eq. (6).

$$\Delta_{\text{sum}}^2 = \sum_{t=0}^{t_e} (C_{\text{test}} - C_{D_i})_{C_2}^2 + \sum_{t=0}^{t_e} (C_{\text{test}} - C_{D_i})_{C_3}^2 \quad (6)$$

C_{D_i} : Gas concentration [mol/mol] in CFD result using diffusion coefficient D_i at time t

C_{test} : Gas concentration [mol/mol] in measurement result at time t

t_e : Specified time [s]

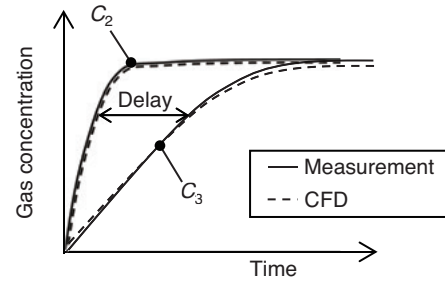


Fig. 7 Image of C_3 gas concentration rise delay against C_2

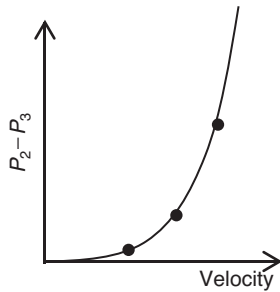


Fig. 5 Gas velocity and filter pressure drop

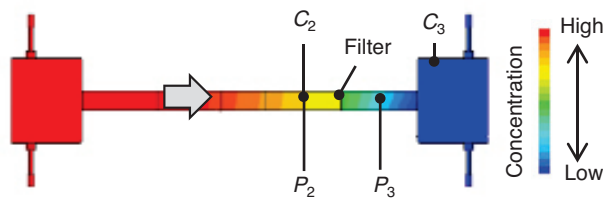
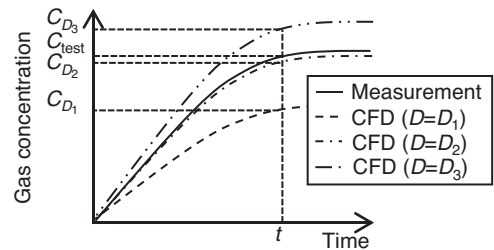
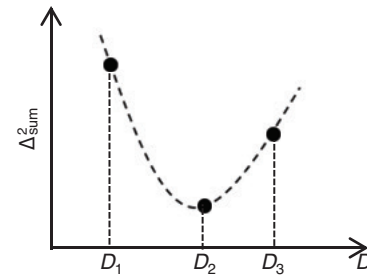


Fig. 6 Image of Gas A concentration distribution



(a) Image of gas concentration profiles with different D_i s



(b) Image of Δ_{sum}^2 against D_i

Fig. 8 Diffusion coefficient identification method

Taking the diffusion coefficient D_i used in each calculation as the horizontal axis and Δ_{sum}^2 from each calculation as the vertical axis, the D that yields the lowest Δ_{sum}^2 was determined.

4. Filter Properties Identification Results and Discussion

4.1. Properties Identification Measurement and CFD Conditions

Table 1 lists the measurement and CFD conditions. The filter used was the TEMISH⁽²⁾ Z3-NTF210SE manufactured by Nitto Denko Corporation. Gas A was a mixture gas of helium (He) and nitrogen (N₂), and Gas B was nitrogen alone to obtain the properties of the mixture gas with helium and nitrogen with respect to the filters.

Gas properties of mixture gas of hydrogen and air were needed for designing the fuel cell system. However, helium instead of hydrogen and nitrogen instead of air were used for safety in this measurement because the flammable concentration threshold of hydrogen was extremely low.

In this measurement, the helium concentration was fixed at 4% and the filter properties were identified from three different Gas A flow results of 5, 10, and 20 cm³/min. The temperature of the room as well as of Gas A and Gas B was fixed at 25°C.

4.2. Solver

FLUENT was used as the solver and transient calculations were carried out. This CFD model has two parts, flow channel and filter, which have their own gas permeabilities. Thus user-defined functions were created to define the mutual diffusion coefficient of mixture gas D_0 to the channel and A_1 , A_2 , and D to the filter. The Chapman-Enskog equation in Eq. (7) was used to calculate D_0 . A_1 and A_2 were given from the measurement and D was given as an assumed value.

The formula for the calculation of D_0 and a list of the variables are shown below.

$$D_0 = \frac{266T^{3/2}}{PM^{1/2}\sigma^2\Omega_D} \quad (7)$$

D_0 : Mutual diffusion coefficient of the mixture gas in the flow channel [m²/s]

M : Molecular weight of the mixture gas [kg/kmol]

σ : Intermolecular potential parameter

Ω_D : Collision integral

T : Temperature [K]

4.3. Identification Results

Figure 9 shows the measurement results of the filter pressure drop $P_2 - P_3$ under three different Gas A flow rates. Dots are the measurement, while the curve was the CFD using identified A_1 and A_2 from the measurement using Eqs.

(4) and (5). The values for A_1 and A_2 were identified through this operation.

Figure 10 shows the results of Δ_{sum}^2 around the identified D . The value for D was identified through this operation.

Using the results of this identification, a comparison was made of the CFD results with the results from measurement of the helium concentrations C_1 , C_2 , and C_3 . Figure 11 shows the results from comparison of concentrations under the three conditions shown in Table 1. The comparison indicated that the CFD results using identified values could satisfactorily reproduce the measured helium concentration profiles under any flow conditions.

4.4. Versatility Check of Identified Results

Versatility of identified filter properties was checked to determine availability to CFD for prediction of filter pressure drop and concentration even under other initial conditions.

Table 2 shows measurements and CFD conditions for verification. Conditions 1 through 3 are for verification related to helium concentration differences. Conditions 4 through 9 are for verification related to gas type using oxygen instead of nitrogen. The identified properties can be checked for their versatility of various flows, concentrations, and gas types.

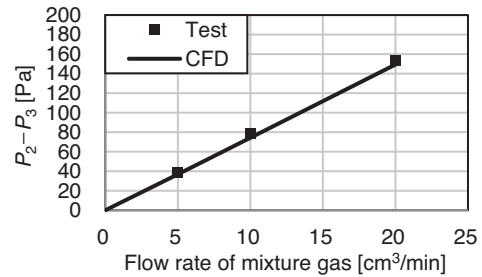


Fig. 9 Comparison of measurement (test) and CFD filter pressure drop with identified A_1 and A_2

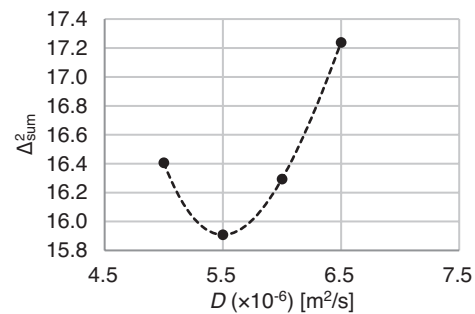


Fig. 10 Δ_{sum}^2 against D_i

Table 1 Measurement and CFD conditions for filter characteristics identification

Gas A				Gas B	Temperature [°C]
He [cm ³ /min]	N ₂ [cm ³ /min]	He+N ₂ [cm ³ /min]	He concentration [%]		
4.8	0.2	5	4	N ₂	25
9.4	0.4	10			
19.2	0.8	20			

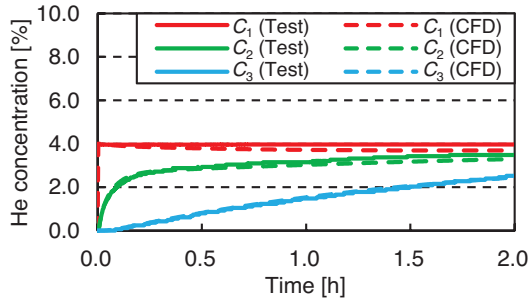
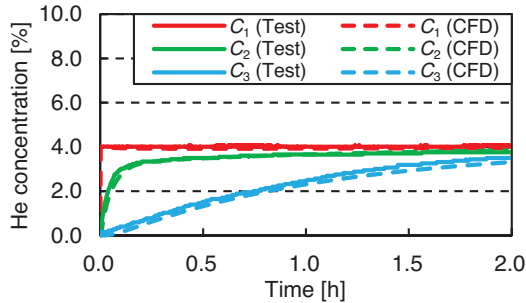
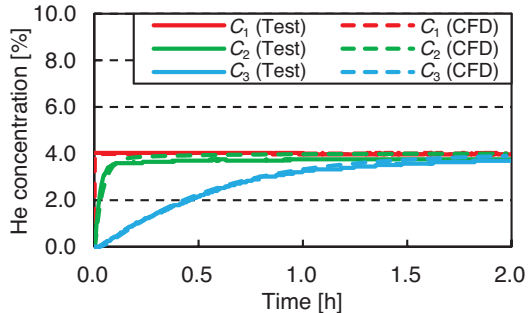
(a) 5 cm³/min(b) 10 cm³/min(c) 20 cm³/minFig. 11 Comparison of measurement (test) and CFD He concentration profiles with identified D at three sensors

Table 2 Measurement and CFD conditions for validation

No.	Gas A				Gas B	Temperature [°C]
	He [cm³/min]	N ₂ [cm³/min]	He+N ₂ [cm³/min]	He concentration [%]		
1	4.6	0.4	5	8	N ₂	25
2	9.2	0.8	10			
3	18.4	1.6	20			
	He [cm³/min]	O ₂ [cm³/min]	He+O ₂ [cm³/min]	He concentration [%]	O ₂	
4	4.8	0.2	5	4		
5	9.4	0.4	10			
6	19.2	0.8	20			
7	4.6	0.2	5	8		
8	9.2	0.4	10			
9	18.4	0.8	20			

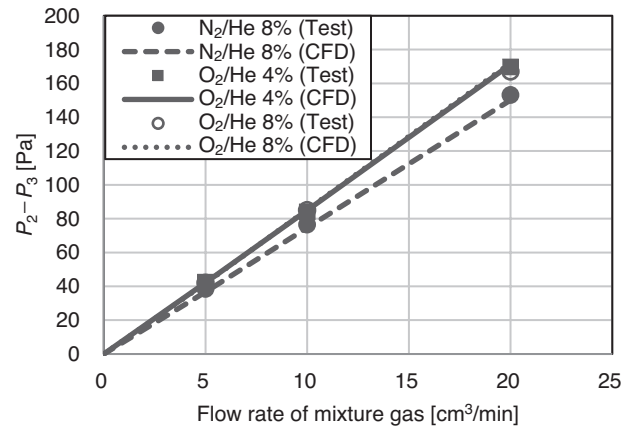
Fig. 12 Comparison of measurement (test) and CFD filter pressure drop with identified A_1 , A_2 , and D

Figure 12 shows the results from comparison of the filter pressure drop measurement values under these nine conditions with the CFD results using the identified values. As shown by these results, it has been confirmed that the identified properties can be used with different concentrations and gas types and still predict the filter pressure drop accurately.

Next, Fig. 13 shows the results from comparison of measurement results and CFD results for concentrations C_1 , C_2 , and C_3 . The CFD results using the identified properties satisfactorily reproduce the measurement results under all conditions.

It was successfully verified that the properties obtained by this method were highly versatile and reliable for use with other concentrations and flow conditions.

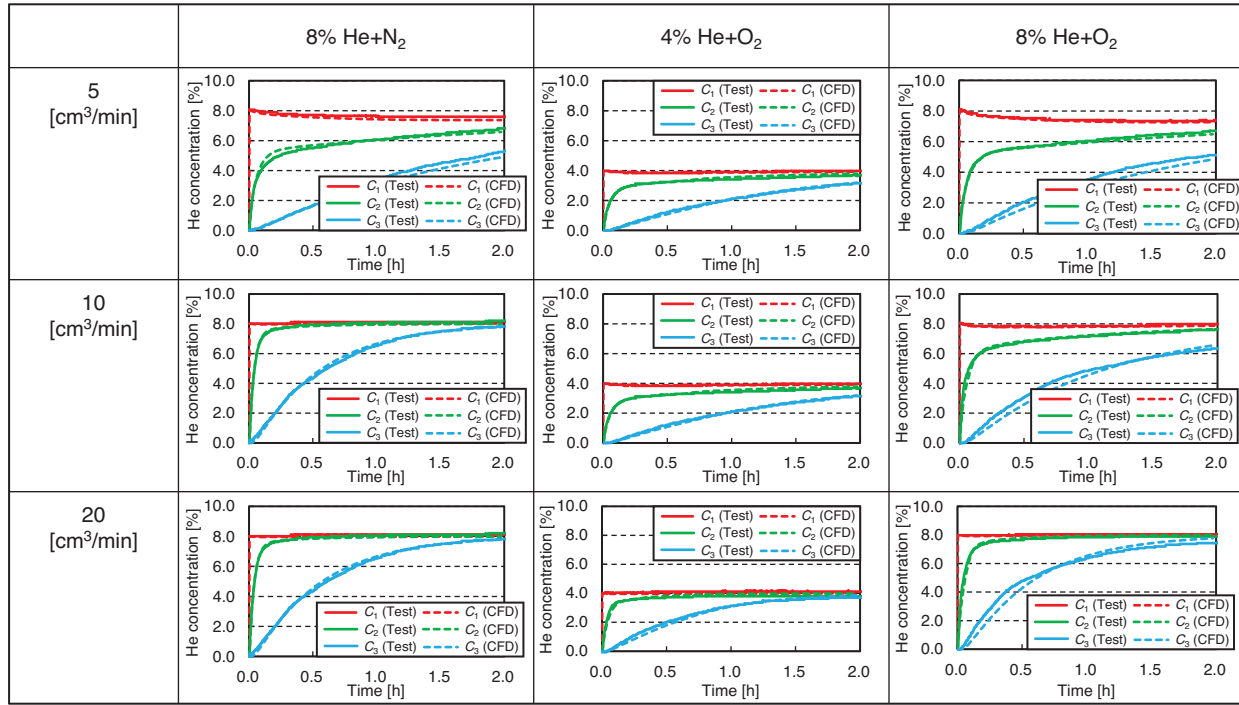


Fig. 13 Comparison of measurement (test) and CFD He concentration profiles with identified D at three sensors for validation

5. Results from Validation of the Design Method

5.1. Overview of Validation

Figure 14 shows a testing apparatus that provides a simple simulation of the hydrogen isolation structure with filters together with a conceptual image of the concentration distribution according to CFD.

The testing apparatus consists of piping for gas inflow, filters with properties obtained in the previous chapter, a box of cuboid shape that simulates the hydrogen isolation structure for the FC stack, and concentration sensors. The inflow of gas is limited to piping at one location only, and helium gas of 100% concentration is made to flow into the box interior from that location. Any other piping and any passages other than the filters are all sealed off. The helium gas that diffuses into the box interior mixes with air as it spreads throughout the whole interior space, then flows out of the box through the filters installed in the sides of the box. When this happens, air also flows into and out of the box through the filters according to the concentration differential between the interior and exterior outside of the box until finally a constant concentration field is created. The helium concentrations at the five locations from Sensor 1 to Sensor 5 in this steady state were measured and validation was performed to determine if these concentrations could be predicted by CFD using the filter properties acquired in the present research.

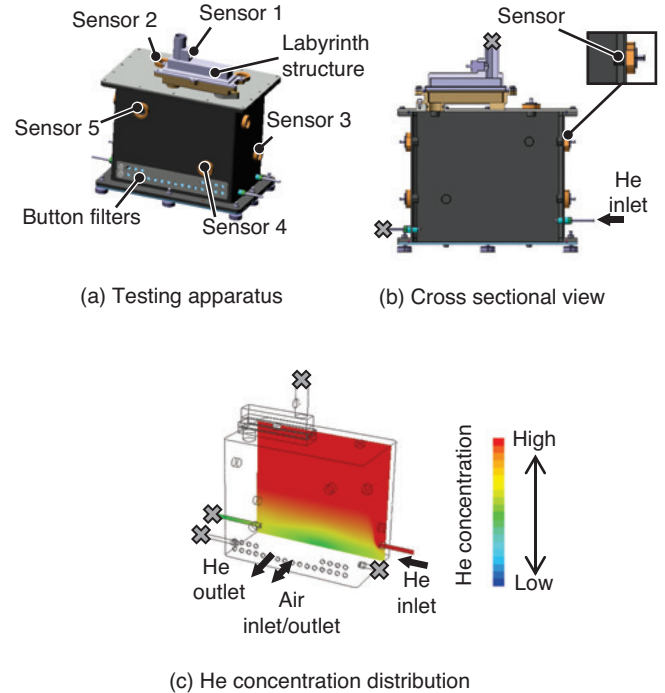


Fig. 14 Testing apparatus and He concentration distribution

Validation was performed under the three conditions shown in Table 3. Condition 1 had no filters so that gas was free to move in and out through 20 filter mounting holes to evaluate CFD performance with extremely low flows. In Conditions 2 and 3, the number of filters and the amount of inlet helium gas were varied from Condition 1 to evaluate the validity of the acquired filter properties and the CFD method. The holes in the portion where filters are not attached under Condition 2 were sealed with aluminum tape. Temperatures were made a uniform 25°C.

5.2. Validation Results

Figure 15 shows a comparison of the results of sensor concentration measurements under every condition with the CFD concentration predicted under the same conditions.

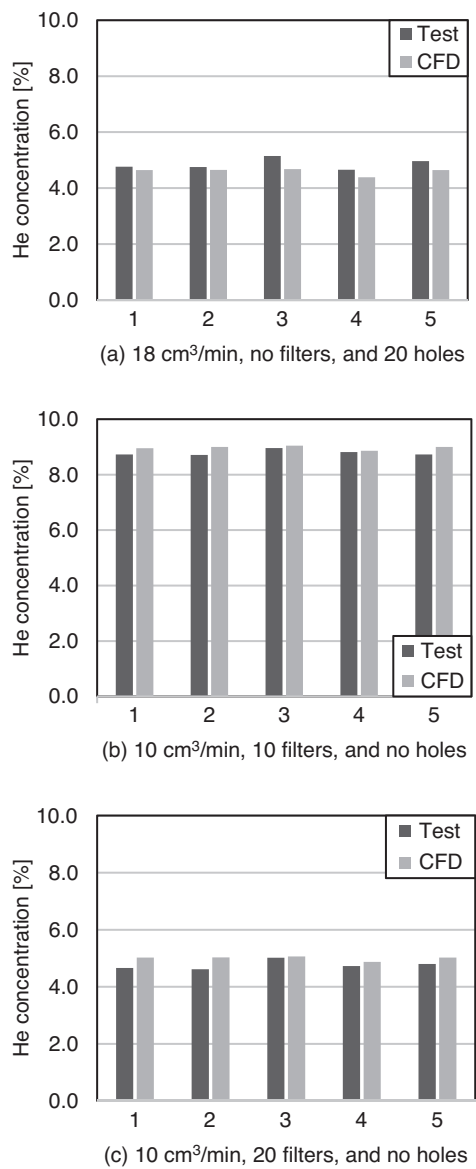


Fig. 15 Comparison of measurement (test) and CFD He concentration at five sensors

Table 3 Measurement and CFD conditions for validation

No.	He [cm ³ /min]	Number of filters	Number of holes
1	18	0	20
2	10	10	0
3	10	20	0

The comparisons in (a) and (c) should have been made at the same flow rate. However, in the test without filters at 10 cm³/min, concentration values below the lower limit guaranteeing sensor accuracy were measured so that the flow in (a) was changed to 18 cm³/min.

The result was that concentrations at high flow without filters were lower than at low flow with filters, and this successfully confirmed that the permeation of air and helium was inhibited by the filters. It was also successfully confirmed in the comparison of (b) and (c) that the fewer the number of filters, the higher the concentration of helium. Although the differences were small in the results for different sensor placement, the simulation successfully reproduced the tendency toward a higher concentration at Sensor 3, near the inlet.

As shown by these results, the CFD results were confirmed to satisfactorily predict the test results under any conditions or sensor locations. This confirmed the validity of the filter properties acquired in the present research and of the CFD method.

6. Conclusion

The results using the filter properties identified by CFD were used to compare the measurements and CFD results under different conditions for validation. Through this research, the design method using CFD for a hydrogen isolation structure with waterproof and dustproof filters was successfully validated.

- (1) The filter properties were identified by measuring gas pressure and concentration on both sides of the filter and then using CFD to reproduce the measurements.
- (2) The design method was confirmed to produce satisfactory prediction even under extremely low gas flow conditions by comparing the gas concentrations from the measurement by a simple testing apparatus to the CFD using identified properties.
- (3) The identified properties were confirmed to be applicable for other initial conditions of gas type, flow, and concentration.

Hydrogen is a flammable gas that is invisible and so it is subject to constraints on location and conditions when testing. A simple method of predicting hydrogen concentrations such as in this research is considered useful in designing a hydrogen isolation structure that is safe as well as compact and light in weight.

This CFD method is also applicable for predicting hydrogen concentrations in an entire fuel cell vehicle, and it can be expected to be an important technology for the realization of a safe hydrogen society.

References

- (1) Kimura, K., Kawasaki, T., Ohmura, T., Atsumi, Y., Shimizu, K.: Development of New Fuel Cell Vehicle CLARITY FUEL CELL, Honda R&D Technical Review, Vol. 28, No. 1, p. 1-8
- (2) https://www.nitto.com/jp/ja/products/temish_search/about/
- (3) JIS K 7126-1: Plastics - Film and sheeting - Determination of gas-transmission rate - Part 1: Differential-pressure method, (2006)
- (4) JIS K 7126-2: Plastics - Film and sheeting - Determination of gas-transmission rate - Part 2: Equal-pressure method, (2006)
- (5) ASTM D1434: Standard Test Method for Determining Gas Permeability Characteristics of Plastic Film and Sheeting, (2015)
- (6) ISO 15105-1: Plastics - Film and sheeting - Determination of gas-transmission rate - Part 1: Differential-pressure methods, (2007)
- (7) JIS P 8117: Paper and board - Determination of air permeance and air resistance (medium range) - Gurley method, (2009)
- (8) JIS L 1096: Testing methods for woven and knitted fabrics, (2010)

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