

Research of Simulation Method of Hydrogen Diffusion for Fuel Cell Electric Vehicle Development

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ABSTRACT

Research was conducted on a method that can simulate hydrogen diffusion behavior in the event that hydrogen leaks into the complexly shaped space around the hydrogen tank of a fuel cell electric vehicle.

Calculations cannot be performed in a permissible time period for the vehicle development with the conventional analysis region partitioning method, so a three-part partitioning calculation method was newly devised to shorten the calculation time. In addition, in order to enhance the calculation accuracy, the turbulence models that can appropriately calculate turbulent diffusion and mixing were selected.

The results confirmed that the peak concentration when hydrogen spouts and the residual concentration after spouting can be calculated at an accuracy of within 5%, while keeping the calculation time to just four days. In addition, it was presumed that the new method can be applied to differing hydrogen spouting conditions. These results indicated that the new method is useful for the development of fuel cell electric vehicles.

1. Introduction

Honda is conducting research and development of hydrogen application technology, such as fuel cell electric vehicles that are the ultimate form of carbon reduction, with the aim of realizing a hydrogen society.

Hydrogen is colorless, odorless, has the lowest specific gravity of all the elements, and diffuses rapidly, characteristics not present in conventional fuels. Therefore, it is important to perform design in consideration of these characteristics.

Hydrogen sensors are installed in fuel cell electric vehicles to detect possible hydrogen leaks (Fig. 1). Conventionally, the installation positions of these sensors were examined using actual vehicles, and it took a few months to determine the positions. If the behavior of hydrogen that flows while diffusing can be analyzed using simulations within a short period of time, the proper

hydrogen sensor positions can be investigated from the design stage.

However, although there have been reports thus far of simulating hydrogen diffusion and verifying accuracy for simple shapes^{(1), (2)}, a survey of research reports in the field of hydrogen application technology finds no examples of proven methods with verified accuracy that can be applied to the design investigation as a simulation method for complex shapes of fuel cell electric vehicles.

Simulations of hydrogen diffusion using complex vehicle shapes have a large calculation scale and it has been challenging to perform the calculations in a practical time so far. Therefore, the method of partitioning the analysis region was modified to shorten the calculation time. In addition, turbulence models that can accurately calculate the turbulent diffusion and mixing of hydrogen were selected to secure an accuracy that enables application to design investigations.

Hydrogen diffusion around the hydrogen tank of a vehicle was simulated using these methods, and accuracy was verified by comparison with measured values obtained by high-speed response concentration measurements.

2. Development Goals

The goal was to construct a simulation method of hydrogen diffusion that can be used to investigate the

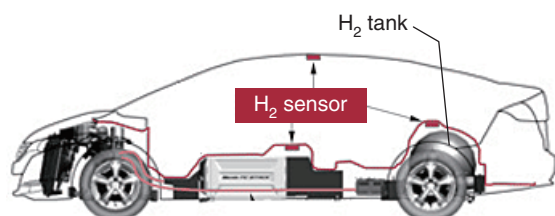


Fig. 1 Position of hydrogen sensors

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design of fuel cell electric vehicles. This entails analysis of changes in the hydrogen concentration over time for a complex vehicle shape, so methods for unsteady state calculations using a 3D space shape that reflects a CATIA model were considered.

The targets for calculation time and accuracy were set as follows:

- (1) Calculation time: One week or less
- (2) Calculation accuracy: Simulated hydrogen concentrations quantitatively match with measured values

The target value for calculation time was set to be advantageous when compared to the time consumed in the investigation of installation positions using conventional tests.

3. Construction of Simulation Method

3.1. Characteristics of Hydrogen Diffusion Phenomena and Issues for Calculation

In the event that hydrogen leaks inside a vehicle, the hydrogen is thought to flow and diffuse through the phenomena shown in Fig. 2. First, jet turbulence that involves compression is formed at the spouting point, and the hydrogen diffuses while rolling up the surrounding air. After that, the flow direction is changed by the structures inside the vehicle, and the behavior shifts to flow and diffusion resulting from wall turbulence due to the effects of the wall surface viscosity. As the flow progresses, the inertia force of the spouting weakens, and the effects of buoyancy become relatively dominant, so the hydrogen rises and remains in the upper areas.

When analyzing these phenomena, the following two issues arise:

- (1) Compressible flow calculations with a high calculation load must be performed using unsteady state calculations with a large number of space meshes and small time steps, which requires longer calculation time; and
- (2) The turbulence models that can accurately analyze the effects of flow and diffusion due to turbulence are unknown.

The first of these issues is described in detail in Section 3.2, and the second in Section 3.3 below.

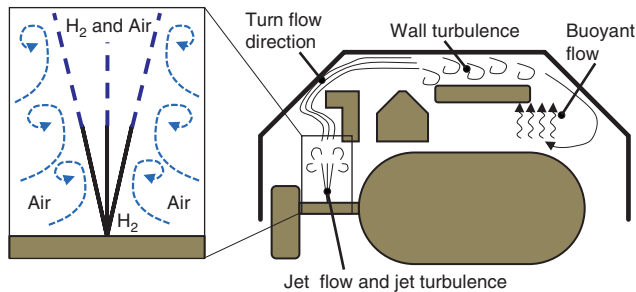


Fig. 2 Flow phenomena in case of hydrogen leak inside vehicle

3.2. Reduction of Calculation Time

3.2.1. Analysis of factors

As described in Section 3.1 above, the reasons for the longer calculation time are the following three points:

- (1) Compressible flow calculations are required
- (2) A larger number of space meshes
- (3) A larger number of time steps

Compressibility affects only the area near the spout, but compressible flow calculations must be performed for the entire analysis area, which increases the calculation load.

The reasons for a larger number of space meshes are that a large number of meshes are required to accurately reproduce the complex shapes inside the entire vehicle, and that even finer meshes are required around the spout to obtain the needed resolution for the jet flow phenomenon.

The reason for a larger number of time steps is that it is necessary to satisfy the courant number restriction in unsteady state calculations. The courant number C is expressed by Eq. (1).

$$C = \frac{v\Delta t}{\Delta x} \quad (1)$$

v : Velocity

Δt : Time step

Δx : Mesh size

The courant number expresses the number of movement meshes of the fluid per time step, and when this number is excessively large, it lowers the accuracy due to value divergence during iterative calculations, or loss of high-frequency components in changes over time. The upper limit value for performing reliable calculations is said to be approximately 40, even when using the implicit method that enables unsteady state calculations with a courant number of 1 or more⁽³⁾. In unsteady state calculations that include the area near the spout where the flow velocity v is high and the mesh size Δx is small, the time step Δt must be reduced to satisfy the courant number restriction. This results in a larger number of time steps.

3.2.2. Conventional technique

The method of imaginary source and the analysis region partitioning method are introduced in “Guidebook on Effective Utilization of H₂” published by the New Energy and Industrial Technology Development Organization (NEDO), as techniques for shortening the calculation time for simulation of hydrogen diffusion⁽⁴⁾.

The method of imaginary source does not calculate the region near the spouting point that requires compressible flow calculations. Instead, it sets the boundary condition using a logical formula for the jet flow from a circular spout, and calculates the remaining regions. It is a challenge to apply this method when there are obstacles near the spouting point, so it is not suitable for the analysis of complex shapes.

The analysis region partitioning method partitions and calculates the region near the spouting point that has a Mach number larger than 0.5 as a compressible flow region, and uses those results as the boundary condition to calculate the remaining incompressible flow region. Compressible flow calculations are limited to only the necessary region, enabling a shorter calculation time. Figure 3 shows the concept of the analysis region partitioning method. Unlike the method of imaginary source, complex space shapes can be reproduced and calculated.

The calculation time was investigated when using the analysis region partitioning method to partition at the Mach number 0.5 position, and performing unsteady state calculations for the second part. In consideration of the sound velocity of hydrogen of 1200 m/s, when the flow velocity v is 600 m/s, the courant number is 40, and the minimum mesh size required to reproduce a complex shape is 5 mm, the time step obtained by Eq. (1) is 3.3×10^{-4} s. Given current computer performance, the calculations for a time of 1 s would require approximately three weeks, even if parallel computing were performed. The aim is to analyze hydrogen diffusion behavior on the order of several seconds to several tens of seconds, so this means that the calculations cannot be performed within the goal of one week.

In order to shorten the calculation time for the second part, the partitioning position was set farther

away from the spout and the flow velocity handled by the unsteady state calculations was reduced. However, the compressible flow calculation area of the first part expanded in this case, so calculations for the first part took one week or more.

3.2.3. Three-part partitioning calculation method

The conventional analysis region partitioning method is unable to avoid the vast amount of the compressible flow calculations in the first part or the unsteady state calculations in the second part. Therefore, a three-part partitioning calculation method was devised that further increases the number of partitions. Figure 4 shows an outline of the three-part partitioning calculation method. In the first part, this method calculates only the area near the spout that requires compressible flow calculations, in the same manner as the conventional analysis region partitioning method. In the second part, incompressible flow steady state calculations are performed for the region up to the position where the courant number in the unsteady state calculations for the third part is 40 or less. The flow velocity at the partition position between the second and third parts should be approximately 10 m/s or less. In the third part, incompressible flow unsteady state calculations are performed for the entire analysis region.

This method was considered to enable the calculations for all analysis regions to be performed in a practical time.

3.3. Enhancement of Turbulence Calculation Accuracy

3.3.1. Turbulence calculation methods

In the diffusion phenomena within a flow field, the effects of turbulent diffusion and mixing whereby mixing is induced by turbulence are more dominant than the effects of molecular diffusion produced by differences in concentration. Methods for calculating turbulence include Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and the Reynolds Averaged Navier-Stokes (RANS) model. DNS and LES precisely calculate all or part of the vortex, so the calculation load is too high, which means that in practical terms it is appropriate to select RANS. Numerous RANS turbulence models have been developed, but there is no all-purpose model yet that can be applied to any calculation subject. This means that to achieve the target simulation accuracy, it is necessary to select models that can accurately calculate each partition calculation region.

Five different turbulence models that have been applied to engineering calculations were taken as candidates, and turbulence models were selected for jet turbulence produced at the spouting point and wall turbulence produced by the flow along a wall surface. Table 1 lists the candidate turbulence models.

3.3.2. Selection of jet turbulence calculation model

The case with a spout diameter of $\phi 1.4$ mm, a flow

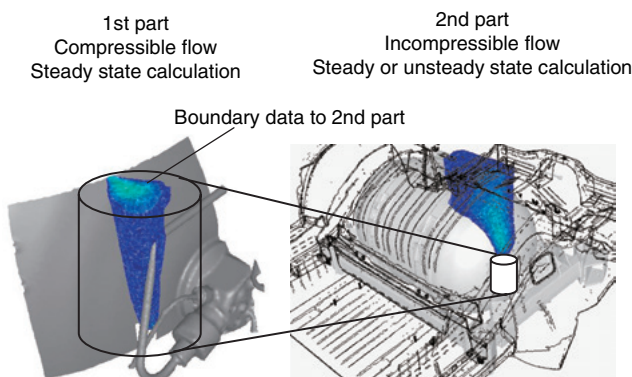


Fig. 3 Analysis region partitioning method

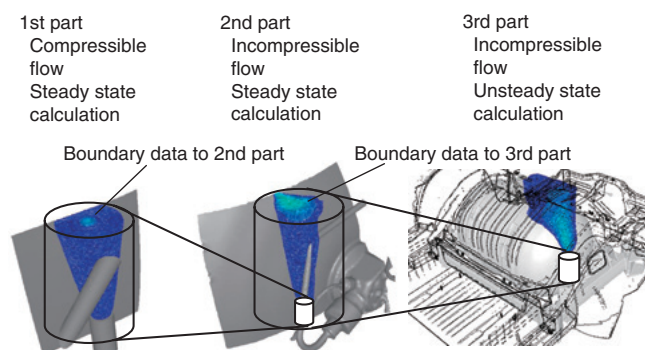


Fig. 4 Three parts partitioning method

Table 1 Turbulence models

Model	Number of equations	Characteristics
k- ω standard	2	Possible to calculate near wall region without wall function
k- ω SST	2	Hybrid model of k- ω standard and k- ϵ standard
k- ϵ standard	2	Basic 2 equations model and popular in engineering field
k- ϵ realizable	2	k- ϵ standard model with enhanced wall function
RSM	7	Possible to calculate turbulent anisotropy

SST : Shear Stress Transport
RSM : Reynolds Stress Model

rate of 120 NL/min, and spouting in the vertically upward direction was verified as a test case. Steady state calculations were performed for the region corresponding to the first and second parts of the three-part partitioning calculation method, and the hydrogen concentration calculated by each turbulence model was compared with the values measured on the spouting axis up to the position 0.2 m from the spout. Figure 5 shows these results.

This shows that the k- ω SST model is the most accurate. In addition, it was verified that hydrogen concentrations can be accurately calculated using the k- ω SST model even when the spouting conditions (spout diameter and flow rate) change. Figure 6 shows these results. The hydrogen concentrations were calculated accurately for any spouting conditions, indicating that the k- ω SST model is valid regardless of the spouting conditions. The effects of jet turbulence are thought to be dominant in the first and second parts of the partitioning calculations, so the k- ω SST model was used for these parts.

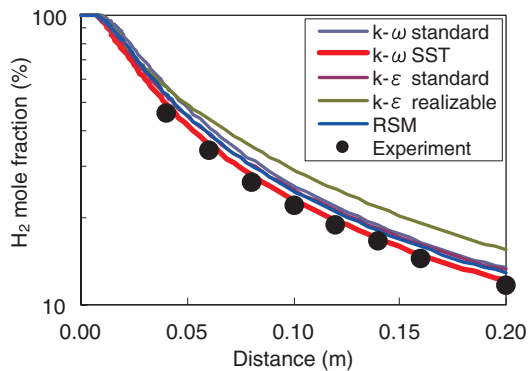


Fig. 5 Comparison of calculations with experiment to select jet turbulence model

3.3.3. Selection of wall turbulence calculation model

Verification was performed for the case with a spout diameter of $\phi 7$ mm, a flow rate of 212 NL/min, and spouting parallel to a horizontal wall surface. The range up to the 0.14 m position on the spouting axis was calculated as the first and second parts of the three-part partitioning calculation method, and the range from 0.14 m to 1 m was calculated using the different turbulence models as the calculations for the third part. Figure 7 shows the results of comparison with the measured values.

The hydrogen concentration values calculated by all of the two equation models for wall turbulence were higher than the measured values, and were unable to adequately express diffusion. On the other hand, the seven equation RSM model matched closely with the measured values. This is thought to be because the RSM model can calculate the anisotropy of the turbulent vortex, so it can express the effects of the longitudinal vortex with strong anisotropy produced by the difference in velocities near the wall surface. Therefore, the RSM model was used for the third part of the partitioning calculations that mainly calculate the flow along the vehicle floor panels.

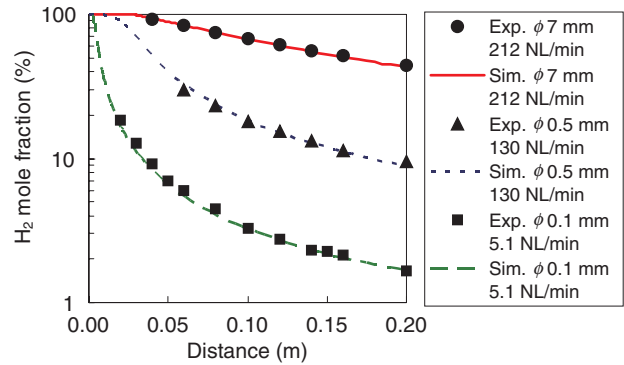


Fig. 6 Comparison of various jet flow calculations with experiments

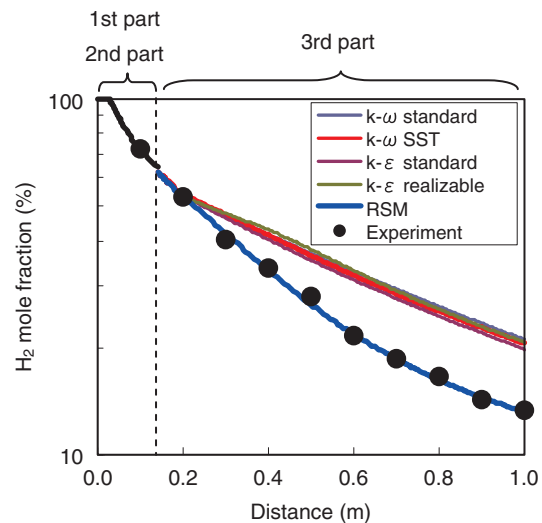


Fig. 7 Comparison of calculations with experiment to select wall turbulence model

4. Method of Verifying the Simulation Method

4.1. Verification Object and Conditions

To confirm the effects of the calculation methods, the calculation time and calculation accuracy were verified by testing and simulating the vehicle underfloor space around the hydrogen tank in a fuel cell electric vehicle in the initial development stage. Typical spouting conditions of a spout diameter of $\phi 7$ mm and a flow rate of 212 NL/min were used. Spouting position was located near the piping joint on the side of the hydrogen tank, and hydrogen was spouted in the vertically upward direction. The spouting time was set at 4 s. Figure 8 shows the hydrogen spouting position and hydrogen concentration evaluation points. Hydrogen concentration evaluation points were set in the three locations of the uppermost point of the floor panel and to the front and rear of that uppermost point.

4.2. Solver

FLUENT6.3 was used as the solver, and the calculations were performed using the implicit method and the SIMPLE (Semi-implicit Method for Pressure-linked Equations)

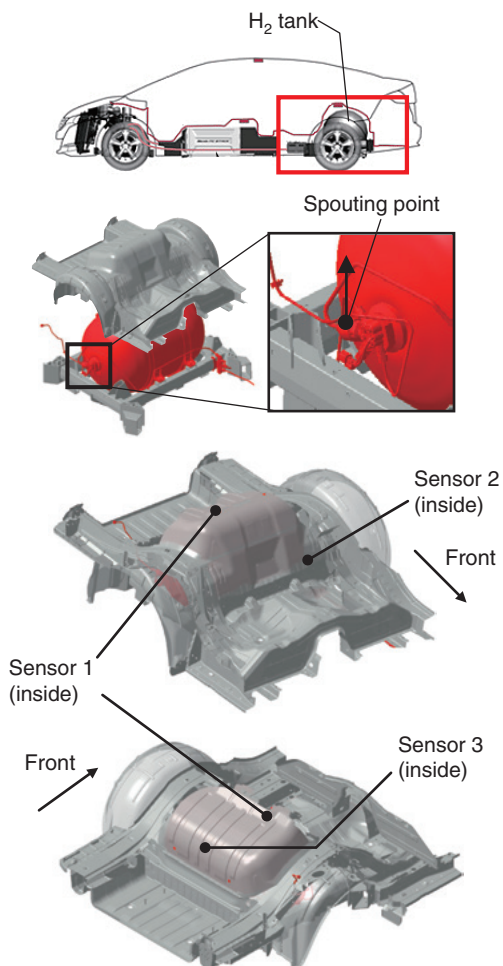


Fig. 8 Model used for experiment

algorithm. A gravity formula was added to the body force item of the Navier-Stokes equation of the model used, to take into account the buoyancy of hydrogen. A Species model based on Fick's diffusion formula that also takes into account turbulent diffusion was used to calculate the hydrogen and air mixing and diffusion.

4.3. Analysis Mesh

The analysis mesh was based on a CATIA model, and was created by first creating surface meshes for each part, then joining these surface meshes, and finally generating the entire space mesh. In order to reproduce the space shapes, the maximum mesh size around each part was 5 mm, and the mesh shape was a tetra mesh.

4.4. Experimental Method

Measurements used hydrogen and vehicle parts corresponding to the CATIA model used for the calculations, and were performed with sufficient care for safety.

Comparative verification of unsteady state calculations for the vehicle underfloor area requires high-speed response and accurate measured values over a wide concentration range. The gas thermal conductivity-type sensors often used to measure hydrogen concentrations over a wide concentration range have a 90% response time of approximately 5 s, which is insufficient for the measurements in this study. Catalytic combustion-type sensors are used to measure concentrations of 4% or less, so these are also not suited for measuring high-concentration hydrogen. Therefore, measurement used the HX-07i ionization detector (made by NOHMI BOSAI LTD.)⁽⁵⁾, which can measure a wide range of hydrogen concentrations and is designed specially for high-speed response measurement.

5. Verification Results

Figure 9 shows the calculation results for each part of the three-part partitioning calculations as hydrogen concentration contour diagrams. The calculation results for the third part enabled visualization of the flow behavior as the hydrogen diffused. The time required for the calculations was one day for the first and second parts, and three days for the third part, for a total of four days, so the calculations could be performed within the target time of one week.

Figure 10 shows the results of comparison with the measured values at each hydrogen concentration evaluation point. The calculated values matched closely with the measured values at each evaluation point. In particular, the concentration at the uppermost point of the floor panel (Sensor 1) could be calculated at an accuracy of within 5% up to 30 s after hydrogen spouting. In addition, the peak concentration and the concentration after 30 s could be calculated at an accuracy of within 5% at the two evaluation points to the front and rear of the floor (Sensors 2 and 3).

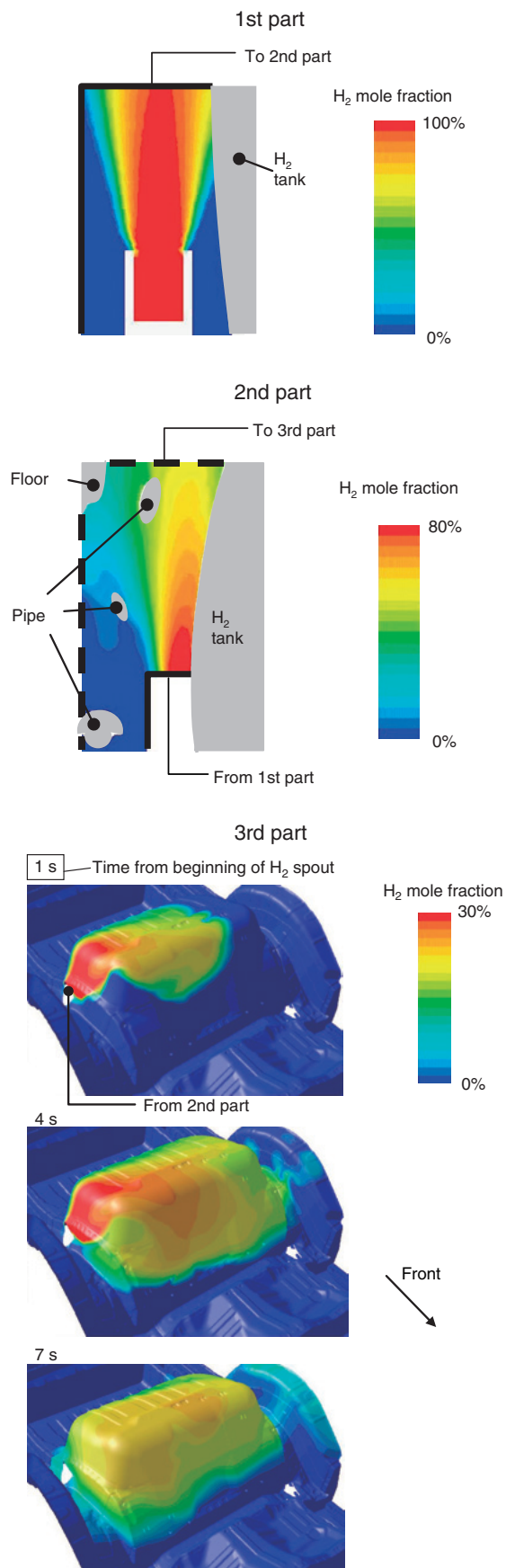
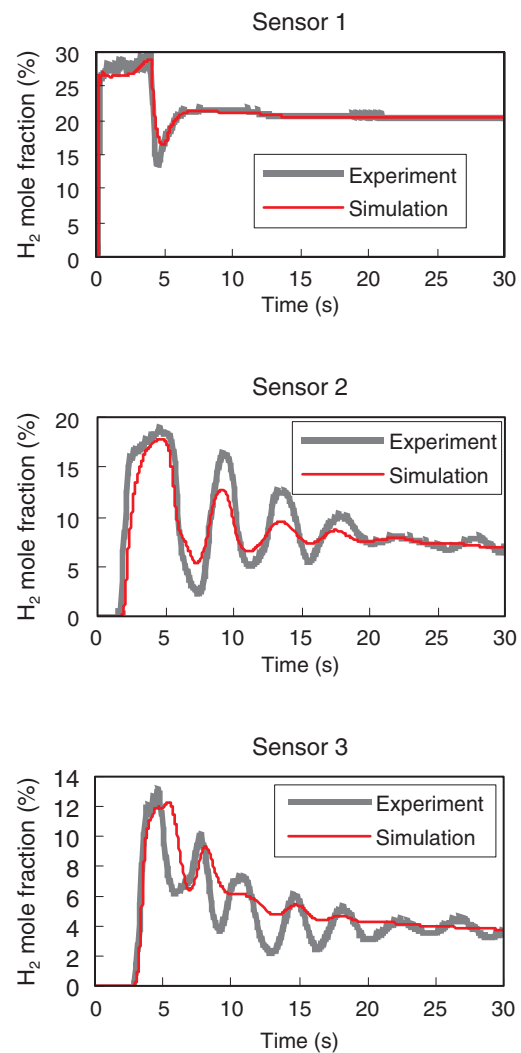


Fig. 9 Hydrogen mole fraction contours


 Fig. 10 H₂ mole fractions at sensor positions

The hydrogen concentration rise time and concentration fluctuation behavior after the end of hydrogen spouting were also closely reproduced.

6. Conclusion

A three-part partitioning calculation method was newly devised as a simulation method of hydrogen diffusion that is useful for investigating the design of fuel cell electric vehicles, and appropriate turbulence models were selected. The effects were verified, and the results confirmed the following two points:

- (1) The calculation time for all regions was four days, which achieved the target of one week or less; and
- (2) The calculated hydrogen peak and residual concentrations matched the measured values within 5%.

It was confirmed that the hydrogen behavior near the spout can be accurately calculated even under differing spouting conditions. The new method showed a wide application prospect for the analysis of various leakage

phenomena inside a vehicle.

High expectations are placed on hydrogen energy for the future of the global environment, and it is desirable to be able to safely handle 'invisible' hydrogen. There are hopes that this study and similar research can help reliably promote technology to make hydrogen more 'visible,' and by using this technology, the authors wish to accelerate the development of vehicles and systems for the control and management of hydrogen.

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