Computational Fluid Dynamics Analysis for Designing Hydrogen Production System

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Hydrogen is expected as the ultimate clean energy that can reduce greenhouse gas emission. In the transportation sector, a fuel cell vehicle (FCV) has been attracting much attention because it is fueled by hydrogen and emits no carbon dioxide. To commercialize hydrogen refueling stations for FCVs, lots of methods to produce hydrogen are being studied. Particularly, on-site hydrogen production from natural gas is one of the most promising methods to supply hydrogen to FCV.

In a previous work, we developed a 40 Nm3/h-class membrane reformer (MRF) system for pure hydrogen production from natural gas with the world highest efficiency of 81.4 %. The MRF system is simpler, more compact and more highly efficient than the conventional Steam Methane Reforming - Pressure Swing Adsorption system; the MRF system makes steam reforming reaction and hydrogen separation process proceed in a single reactor simultaneously. More compact and more efficient system is, however, desired to realize a cost competitive hydrogen refueling station. To meet this requirement, we developed a new-concept hydrogen production module with membrane on catalyst (MOC). In the MOC concept, a porous support itself has the activity of reforming catalyst as well as the role of structural membrane support (Fig. 1), while the conventional MRF system requires a separate catalyst. Therefore, the MOC module can provide a more downsized hydrogen production system than the conventional system. Concerning the performance, we demonstrated that the MOC module has hydrogen production efficiency comparable to the MRF system. However, the MOC module is potentially more efficient because it employs membrane with higher hydrogen permeance than the MRF system. The MOC module will be more efficient if we can optimize its shape, design and operation conditions.

In the present study, we conducted a computational fluid dynamics (CFD) simulation for the MOC module considering chemical reactions and mass transport. The simulation was based on assumptions as follows: 1) A temperature distribution was uniform. 2) Rate of the reforming reaction was infinite. 3) Hydrogen permeation was proportional to differential square root of hydrogen pressures across the membrane (Sievert’s law). 4) Gas flux in the porous support was proportional to pressure drop and inversely proportional to viscosity (Darcy’s law). Through the CFD simulation, we evaluated the product hydrogen flux, the hydrogen recovery and the methane conversion under standard operation conditions for the MOC module as follows: 1) Natural gas input flow rate was 0.28 NL/min (2.1×10^{-4} mol/sec). 2) Steam to Carbon ratio of the input gases was set at 3.0. 3) Operation temperature was 500-550 deg C. 4) Pressure of the process side (inside the MOC module) was 0.8 MPaG. 5) Pressure of the permeate side (outside the MOC module) was 0.0 MPaG. The simulation results of the product hydrogen flux, the hydrogen recovery and the methane conversion were in good agreement with the experimental results under the same operation conditions.

Among the simulation results, we focused on hydrogen concentration profile in the MOC module and heat flux through the catalyst. The CFD simulation shows that the hydrogen concentration in the porous support adjacent to the membrane is lower than that in the free space between the insert tube and the porous support (Fig. 2). Furthermore, hydrogen partial pressure is dramatically varied spatially by the existence of the porous support. In other words, significant concentration polarization occurs in the porous support. To overcome this problem, we have a possibility to enhance the hydrogen production of the MOC module by optimizing its shape design and operating conditions to reduce the gas phase resistance in the porous support. For example, the CFD simulation shows that we can improve hydrogen production by changing the length and shapes of the insert tube inside the MOC module. From the simulation result of the heat flux distribution on the catalyst, we found that stronger endothermic reaction occurred and much more hydrogen was produced near the closed end than any other positions of the MOC module.

In addition to the single MOC module, we conducted a CFD simulation for a MOC reformer, which was a gas-fired reformer equipped with multiple MOC modules. We developed a small-scale MOC reformer containing twelve MOC modules for demonstration, while a large-scale MOC reformer containing thousands of MOC modules will be required for practical use. In the future work, we will optimize the shape design and operating conditions for the MOC reformer system as well as the single MOC module using the CFD simulation.

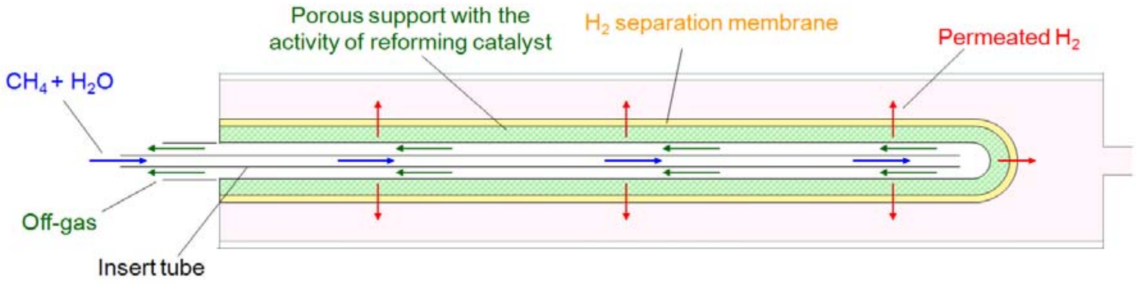

Fig.1 Schematic Diagram of the MOC module

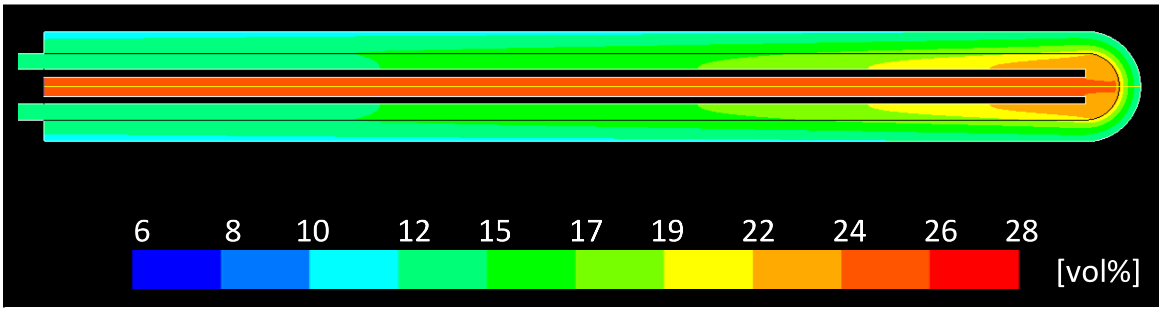

Fig.2 Concentration distribution of H_2 in the MOC module

(T=550degC, P=0.8/0.0 MPaG, Input: Natural Gas=3.0 Nml/min/cm^2, Steam to Carbon ratio =3.0)