

Particle Design Based on the Structural and Molecular Diffusion Characteristics of TWC Aggregates with Connected Pores

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In recent years, while the transition to zero-emission vehicles has progressed, it is expected that internal combustion engines and hybrid vehicles will continue to be used during the transitional period toward full zero emissions. There is a growing need for advanced exhaust gas purification technologies. The authors have developed TWC particle membrane filters that integrate GPF and TWC, achieving space-saving in post-treatment equipment. Furthermore, by using porous particles with communication holes inside TWC particles, the material diffusion coefficient is improved, enabling low-temperature CO purification. This study aimed to clarify the impact of the internal pore structure of TWC porous particles on diffusion phenomena. Using a porous model representing the internal structure of TWC porous particles, we evaluated the diffusion coefficient when pore diameter and mean free path changed and examined guidelines for highly efficient catalyst design.

A cube with 800 voxels on one side is given a void, and the diffusion coefficient analyses were performed. The diffusion simulation employed a random walk method that considers intermolecular collisions and collisions between molecules and walls. The number of molecules to be injected was determined so that the maximum relative standard deviation of displacement was less than 0.01, and the molecular diffusion coefficient D were calculated using the following formula. Here, $E[...]$ is the expected value, $\mathbf{x}_t$ is the particle position at time t , $\mathbf{x}_0$ is the initial particle position, and ε is porosity.

$$\mathbf{D} = \frac{E[(\mathbf{x}_t - \mathbf{x}_0)(\mathbf{x}_t - \mathbf{x}_0)^T]}{2t} \quad (1)$$

Figure 1 shows the relationship between the diffusion coefficient and pore diameter when voxel size is changed. By doubling the voxel size, the calculation area is doubled. For cubes with a voxel size of 1 nm and a calculation area of 800 nm, the diffusion coefficient remained generally constant at the pore diameter of 200 nm ~ 300 nm and increased again after the pore diameter of 300 nm. This is presumed to be because the computational area relative to the pore size was insufficient, causing bias in the pore arrangement, and local cavity connection states and the distance between cavities affected the diffusion coefficient. On the other hand, the voxel size of 2 nm for cubes with a computational area of 1600 nm, the diffusion coefficient increased almost linearly up to a pore diameter of 400 nm. Therefore, it was determined that the computational area was sufficient for structural evaluation up to a pore diameter of 400 nm, and thereafter the conditions of voxel size 2 nm and 1600 nm cubic area were adopted.

Figure 2 shows the relationship between diffusion coefficient and pore diameter when the mean free path is changed to 50nm, 100nm, and 150nm. At 50nm, the average increase rate at 50nm intervals was 16.8%, while at 150nm, the average increase rate was 26.4%. It was confirmed that the longer the mean free path, the higher the increase rate of diffusion coefficient.

Based on the results of this study, by appropriately selecting the computational area, it is possible to It was shown that the diffusion coefficient increases linearly. Additionally, by varying the mean free path, it was confirmed that the longer the mean free stroke, the greater the rate of increase in the diffusion coefficient. On the other hand, increasing the pore diameter reduces the specific surface area of the catalyst, so it is necessary to consider the balance between the diffusion coefficient and specific surface area. Going forward, we plan to conduct reaction rate analysis and investigate the optimal internal structure that contributes to improving reaction rate.

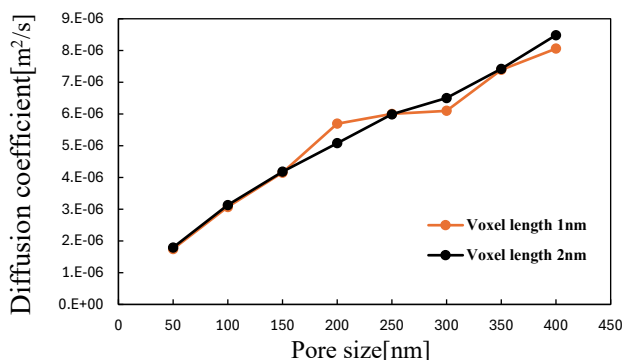


Fig.1 Effective Diffusivity for Different Domain Sizes

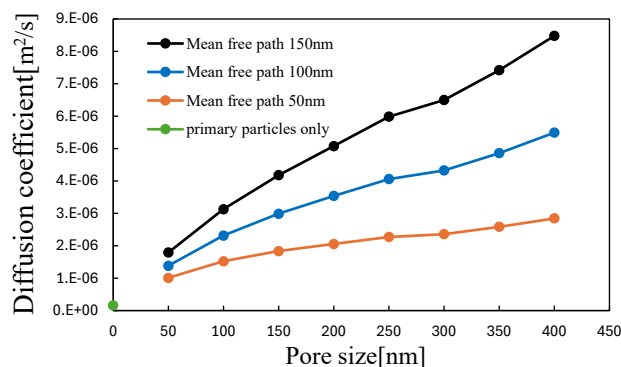


Fig.2 Effective Diffusivity for Different Mean Free Paths