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A discrete particle packing model for the formation of a catalyst layer in polymer electrolyte fuel cells

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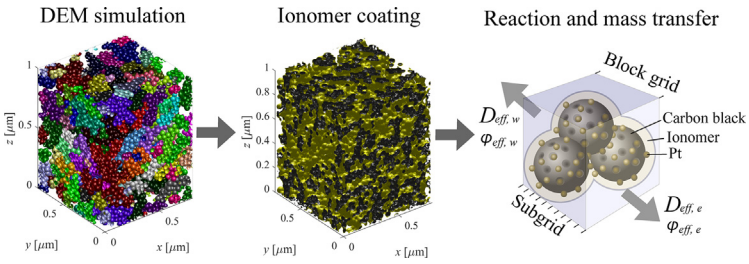
HIGHLIGHTS

- A model of a fuel cell catalyst was developed based on packing of agglomerates.
- Electrochemical reaction and mass transfer was simulated on the resulting geometry.
- Branched agglomerates resulted in a higher porosity and increased pore size.
- The agglomerate size increased oxygen void diffusion but reduced proton conduction.
- This study can increase our understanding to improve the fuel cell performance.

GRAPHICAL ABSTRACT



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ABSTRACT

We developed a reconstruction simulation model for a catalyst layer of a polymer electrolyte fuel cell to elucidate the effect of the size and shape of the catalyst agglomerates on the cell performance. The geometry of the catalyst layer was obtained by simulating the packing of carbon black agglomerates in ink modeled as multisphere objects by the discrete element method. Electrochemical reaction and mass transfer were modeled based on the resulting three-dimensional geometry of the catalyst. Both the size and shape of the agglomerate significantly influence the catalyst structure and performance. Branched agglomerates lead to higher porosity, larger pore sizes, and better cell performance. For each agglomerate shape, there is an optimum size at which the performance is the maximum, because of the optimum trade-off relationship between the oxygen diffusion and proton

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