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The effect of solvent and ionomer on agglomeration in fuel cell catalyst inks: Simulation by the Discrete Element Method

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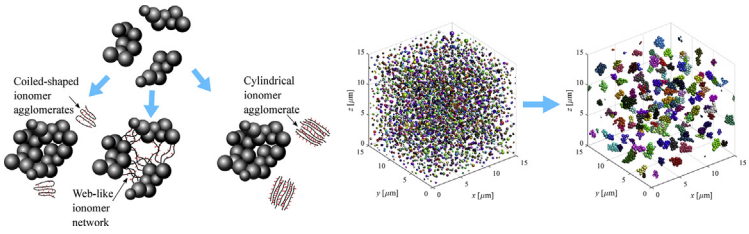
HIGHLIGHTS

- A particle model to simulate agglomeration in fuel cell catalyst ink was developed.
- It comprises a new model of steric force due to ionomer between carbon aggregates.
- This force was modelled as a function of the dielectric constant of the solvent.
- The model can predict the agglomerate sizes observed in various ink experiments.
- It can be utilized to optimize the solvent for best catalyst porous structures.

GRAPHICAL ABSTRACT



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ABSTRACT

We simulate agglomeration in different fuel cell catalyst ink solutions using Discrete Element Method. Carbon support is modelled as particles in various inks with ionomer and various solvents. The particles interact with particle-pair forces resulting in agglomerate build-up. The classical colloidal theory with van der Waals and electric double layer forces underestimates the ink stability, which motivates the development of a new model of polymer force between particles. The force is activated when there is a bridging of polymer between the carbon black particles, and the strength is dependent on the ionomer interaction with the solvent by the dielectric constant. A critical dielectric constant was defined for which ionomer form a web-like polymer network that increases the ink stability. This modification can explain the trend of the ink stability, and the model can simulate the

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