Predicting of pressure acting on the electrode surface based on continuum approach

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Recently, the sizes of electrochemical systems become small and they are being integrated in order to achieve high power density. Also the electrode design has been changed to the nano-porous structure to increase the area of contact surface without changing the size of system. When it comes to the nano-scale, the physical phenomenon, such as Electric Double Layer (EDL) overlapping or electro-capillarity phenomena could occur, which is not existing at the bulk-scale. EDL overlapping phenomena could affect the pressure acting on the surface and the exerted pressure is related to the stability of systems.

In this study, by adopting both atomistic approach (MD simulation) and continuum approach (equation based model), we calculated the pressure acting on the electrode surface and compared the pressure calculated from both approaches. Although, in small length scales, the atomistic approach is known as more appropriate for describing ion distributions than the continuum approach, we found that the continuum based model could also be used in small length scales, and the predicted results showed good agreement with MD results.