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Investigating charged nanoparticles diffusion in brain tumour microstructures at pore-scale

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Nanoparticles (NPs) have emerged as promising candidates for targeted drug delivery in the treatment of brain tumours due to their diverse physicochemical properties. With the advanced development of convection-enhanced delivery (CED), anticancer drugs are directly infused into the targeted brain tumour region through a catheter, enabling drugs to bypass the blood-brain barrier (BBB). Multiple factors, such as particle size and surface charge are crucial for enhancing the NP transport in brain tumours [1]. However, primarily owing to the complex microstructure and microenvironment of the brain tumours, how these physical properties affect the NPs diffusion in the brain tumour at pore-scale still needs to be clarified and quantified.

In this study, we first established a framework consisting of different geometrical models of brain tumour microstructures from Grades 1-4 [2] and the particle tracing model to investigate the relation between the effective NP diffusion coefficient in brain tumours and their physical properties. We verified the predictive power of the present model by comparing the results under the same conditions to experimental results reported in the literature [1]. Then, we quantitatively analysed the NP diffusion coefficient in order to establish the effect of particle size, surface charge, temperature and extracellular matrix. We found that the diffusion coefficients of NPs are positively related to all these physical properties when the total surface charge increases with the particle size [3]. Conversely, the diffusion coefficient of NPs negatively corresponds to the particle size when the total surface charge is kept the same. The magnitude of the diffusion coefficient with the zeta potential (Z_p) of -5mV is at least 1500 times larger than that value of uncharged NPs. This difference is even more pronounced with larger NP sizes. More interestingly, we noted that the diffusion coefficient in the high-grade tumour microstructures is smaller than that in low-grade tumour microstructures when other parameters are kept the same, although the high-grade tumours possess a higher porosity than low-grade tumours. This may imply that higher level of hyaluronic acid (HA) of ECM deposited within the interstitial fluid is essential for the critically decreased diffusion coefficient in high-grade tumours.

Results from this study can deepen the understanding of the relationships between NP diffusion coefficient and physical characteristics of NPs in brain tumours, providing crucial insights and a reliable modelling framework for the development of nano-drugs and carrier delivery processes in chemotherapy of brain tumours and other brain disorders.

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