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ON THE EFFECT OF CAPPING THE ENDS OF CARBON NANOTUBES USED FOR DRUG DELIVERY

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Abstract. In practice a sealed capsule may be required for targeted drug delivery systems to maintain the drug molecules inside before release at the target cell. In this note, applied mathematical modelling is undertaken in an attempt to understand the effect of capping the ends of a carbon nanotube. Here we envisage a titanium dioxide nanoparticle to be the drug molecule and a single-walled carbon nanotube is supposed to be the capsule. The Lennard-Jones potential function and the continuous approximation are utilized to determine the molecular interaction energy of the system. For convenience, throughout this analysis we assume that all configurations are in a vacuum and that the titanium dioxide nanoparticle is symmetrically located along the axis of the nanotube and is initially at rest. As might be anticipated, the upshot is that capped ends are necessary in order to minimise the molecular interactions which enhance the overall stability of the confined system.

Keywords. Carbon nanotube, Capping ends, Lennard-Jones potential, Continuous approximation, Drug delivery.

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