B**oundary Effects in the Hexagonal Packing of Rod-like Molecules Inside a Right Circular Cylindrical Domain I. The case of right circular spherocylindrical molecules**

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Abstract
We derive an upper limit, imposed by cinematic constraints, for the ratio of the average density function relative to the local density function for a freely rotating right circular cylindrical domain made of right circular spherocylindrical molecules. The derivation is made under the assumption that the molecules are ridgid, that they are close packed and that their molecular axes are perpendicular to the base of the domain. For domains containing more than 100 molecules, the avarage density, evaluated as a function of domain size, is well approximated by a simple smooth analytical expression. For smaller domains, on the other hand, the boundary effects lead to an average density that varies erratically with the size of the domain. The contribution of the boundary effects to the difference between the local density and the average domain density, increases with decreasing domain size. It is negligible for very large domains, it is about 2.5&perc; for domains containing around 10 000 molecules; and it can be as high as 20&perc; for very small domains. The theoretical results obtaied here are consistent with the reported discrepancy between the value of the molecular area obtained from pressure area measurements and that obtained from X-ray measurements.