

Boundary effects in the Hexagonal Packing of Rod-like Molecules Inside a Right Circular Cylindrical Domain II. The case of inclined spherocylindrical molecules

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Abstract We derive an upper limit, imposed by cinematic constraints, for the packing fraction of right circular spherocylindrical molecules inside a freely rotating right circular cylindrical domain at a gas-liquid interface. The derivation is made under the assumption that the molecules are rigid and close packed. The expression obtained for the packing fraction as a function of domain size and angle of inclination is exact for all domain sizes and all values of the inclination angle. For small angles of inclination ($< 20^\circ$), and domains containing more than 30 molecules, the packing fraction can be approximated by a simple smooth analytical expression. The domain size at which the approximation is reasonable increases with increasing angle of inclination. At an inclination angle of 40° the approximation is good for domains containing 300 molecules or more.