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Studies on the Relationship Between the Local Pressure Tensor Field and the Forces Acting on Particles in Simple Molecular Models J. MATTHEW MANSELL, North Carolina State University — Over the past decade, numerous research efforts have resulted in a growing body of evidence indicating that components of the local pressure tensor field attain values of very large magnitude in many nanopore-adsorbate systems, and that many unique properties of these systems can be explained by these large-magnitude values. Here, I present results of computational measurements of the local pressure field (using the Irving-Kirkwood definition), as well as the mean compressive force acting on particles, in a series of typical nanopore-adsorbate models, as well as in bulk fluids. In agreement with the works mentioned above, I find that certain components of the local pressure field in the pore-adsorbate systems indeed attain extrema with very large magnitudes, whereas the magnitudes of the extrema in the bulk systems are much smaller. I also find that the average compressive forces acting on the particles in either type of system are very similar. Hence, although the local pressure can be very high in the nanopore-adsorbate systems, this does not suggest that the compressive forces acting on the particles in those systems is significantly larger than in bulk fluids, contrary to the nave interpretation.

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