Normal Pressure Coefficients from Poiseuille Flow, SLLOD Dynamics and the Coleman-Markovitz Relation

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Normal pressure differences are important in many different rheological applications, but their effects in microfluidic and nanofluidic flows have not been studied. Microfluidic flows are usually modelled using linear transport theory, but it is clear that nonlinear effects will become increasingly important as more complex fluids are studied. We have computed the local volume averaged pressure as a function of position for a polymer solution in Poiseuille flow, and used the results to obtain the first normal stress coefficient as a function of position. The value of the zero shear rate normal stress coefficient that we obtain is consistent with that computed by zero shear rate extrapolation of the shear rate dependent normal stress coefficient from the SLLOD homogeneous shear algorithm. It is also consistent with the value obtained from the Coleman-Markovitz relation using the shear relaxation modulus computed from the Green-Kubo formula with equilibrium molecular dynamics. In principle, the remarkable agreement between the results of these three independent computations can be understood by applying nonlinear response theory. An outline of a possible proof will be given, along with a discussion of some contentious points that arise along the way.