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Number Dependence of Viscosity in Two Dimensional Fluids

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NOTE

NUMBER DEPENDENCE OF VISCOSITY IN TWO DIMENSIONAL FLUIDS

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Mode coupling theory [1] predicts that in two dimensions for sufficiently large system size, the shear rate, $\dot{\gamma}$, dependent viscosity, $\eta(\dot{\gamma})$ should vary as, $\eta(\dot{\gamma}) \sim \log(\dot{\gamma})$ for sufficiently small $\dot{\gamma}$. Similarly the hydrostatic pressure, p , is predicted to behave as $p(\dot{\gamma}) \sim \dot{\gamma} \log \dot{\gamma}$.

In early work [2] with small systems, $N < 100$, we did indeed observe results that were apparently consistent with these predictions. However later data obtained with faster computers on larger systems, $N < 3500$, showed quite different behaviour [3]. The large system results were quite similar to those for small systems at high shear rates but at low shear rates the viscosity of the large systems was essentially independent of shear rate rather than diverging logarithmically as predicted by mode coupling theory.

It has been proposed however that the fluctuations described by mode coupling theory and which would lead to a logarithmic divergence of the two dimensional viscosity, may be unstable [3]. This would seem a definite possibility in that mode coupling theory predicts [1] that at low strain rates the hydrostatic pressure, p , should be *less* than the corresponding equilibrium pressure.

Because of the theoretical importance of this data and because of the large number dependence previously observed, it is clearly important to establish the behaviour of these rheological functions for even larger systems. In this short note we show results for systems ranging in size from $N = 32$ to $N = 57,344$.

We studied systems of soft discs which interact via the potential, $\phi(r) = \epsilon(\sigma/r)^{12}$. A cut-off distance of 1.5σ was employed and the temperature and number density were: $kT/\epsilon = 1.0$ and $n = 0.9238\sigma^2$, respectively. Throughout the following we will use reduced units in which all physical quantities are expressed in terms of the soft disk potential parameters, σ , ϵ , and the particle

Table 1 Shows the shear viscosity and the hydrostatic pressure for soft discs as a function of system size and strain rate.

$\gamma\dot{N}$	57344	14336	896	224	98	72	56	32
0.01	3.8 ± 0.1	3.87 ± 0.03			3.74 ± 0.05	4.07 ± 0.03	4.84 ± 0.09	
0.01778		3.85 ± 0.02			3.73 ± 0.04	4.07 ± 0.04	4.62 ± 0.05	
0.0316		3.82 ± 0.02	3.84 ± 0.03	3.75 ± 0.06	3.72 ± 0.03	3.82 ± 0.05	4.29 ± 0.05	5.17 ± 0.06
0.057		3.78 ± 0.01			3.59 ± 0.04	3.67 ± 0.02	3.91 ± 0.02	
0.1	3.65 ± 0.02	3.63 ± 0.02	3.66 ± 0.03	3.58 ± 0.01				4.06 ± 0.01
0.1778		3.42 ± 0.01		3.41 ± 0.01				
0.316		3.11 ± 0.01		3.12 ± 0.02	3.08 ± 0.01	3.13 ± 0.01	3.19 ± 0.01	3.21 ± 0.02
0.57	2.763 ± 0.004							
1.0	2.401 ± 0.002	2.392 ± 0.003	2.395 ± 0.001		2.74 ± 0.01	2.41 ± 0.01	2.42 ± 0.01	2.47 ± 0.01
Pressure								
0.0		10.895 ± 0.001		10.913 ± 0.003	10.952 ± 0.001	10.907 ± 0.001	10.844 ± 0.005	11.009 ± 0.001
0.01	10.895 ± 0.001	10.895 ± 0.001						
0.01778		10.896 ± 0.001			10.942 ± 0.001	10.899 ± 0.001	10.842 ± 0.003	
0.0316		10.899 ± 0.001	10.900 ± 0.001	10.917 ± 0.002	10.946 ± 0.001	10.906 ± 0.003	10.859 ± 0.002	10.864 ± 0.003
0.057		10.910 ± 0.001			10.955 ± 0.001	10.923 ± 0.001	10.887 ± 0.003	
0.1	10.932 ± 0.001	10.935 ± 0.001	10.933 ± 0.001	10.953 ± 0.001	10.982 ± 0.001	10.957 ± 0.001	10.934 ± 0.002	10.963 ± 0.002
0.1778		10.995 ± 0.001		11.009 ± 0.002				
0.316		11.124 ± 0.002		11.133 ± 0.004	11.155 ± 0.001	11.160 ± 0.002	11.168 ± 0.001	11.209 ± 0.002
0.57	11.399 ± 0.002							
1.0	11.956 ± 0.003	11.941 ± 0.001	11.952 ± 0.001		11.994 ± 0.002	12.013 ± 0.004	12.043 ± 0.002	12.145 ± 0.005

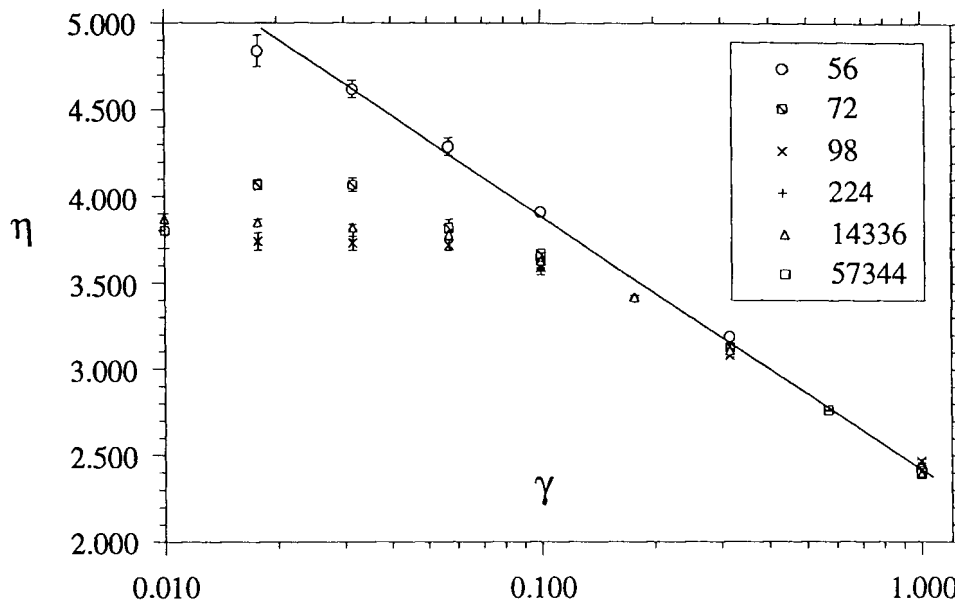


Figure 1 Shows a subset of our shear viscosity data for the state point $n = 0.9238$, $T = 1.0$. For $N > \sim 200$ the viscosity coefficient is remarkably independent of system size, N . For large N and small strain rates, γ , the viscosity is, within statistical uncertainties, independent of strain rate.

mass, m . The algorithm was the standard Gaussian thermostatted SLLOD method for planar Couette flow [4].

Table 1 shows the shear viscosity, η , and the hydrostatic pressure, ($p \equiv \frac{1}{2}(P_{xx} + P_{yy})$), as a function of both the system size, indicated by the number of particles, N , and the strain rate, γ . Figure 1 displays a subset of the viscosity data. As can be seen from both Table 1 and Figure 1, for $N > \sim 100$, $\eta(\gamma, N)$ is independent of N . For $\gamma < \sim 0.1$ and $N > \sim 100$ the viscosity is independent of strain rate. For small N the viscosity is consistent with a logarithmic function of strain rate. For larger values of N the viscosity appears to be both independent of N and γ at low strain rates.

Figure 2 shows a subset of the hydrostatic pressure data. In this Figure we plot the shear induced shift in the hydrostatic pressure divided by the strain rate, as a function of the logarithm of the strain rate. The mode coupling prediction would appear as a straight line on this graph. As can be seen, the $N = 98$, $N = 72$ results are apparently consistent with this behaviour. These small system results are new and were obtained from extremely long, 20 million timestep, runs. Although in agreement with older work on small systems [2], these results are really quite surprising. They show that at fixed N, V, T , for these small systems at low shear rates, the hydrostatic pressure away from equilibrium can be *less* than the corresponding equilibrium value. From Table 1, we can see that this phenomena can also be seen for the $N = 98, 72, 56, 32$ systems, although the maximum shear rate at which this negative shear dilatancy is observed does vary somewhat with system size.

Comparing Figures 1, 2, we see that the N, γ regime where negative shear dilatancy is observed does not correspond to the regime in which the viscosity is

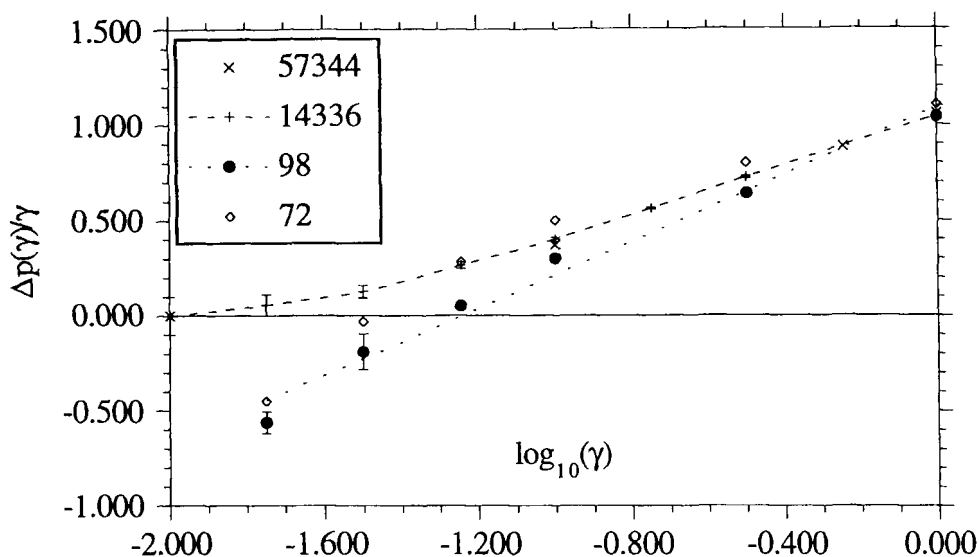


Figure 2 Shows a subset of our hydrostatic pressure data for the same state points as in Figure 1. $\Delta p(\gamma)$ denotes the difference, $p(\gamma) - p(0)$ for each specific system size. For small systems and shear rates the systems display *negative* shear dilatancy. For the larger systems only positive dilatancy is observed.

independent of strain rate and N . In Figure 1, the $N = 98$ system seems to clearly exhibit shear turn-over behaviour similar to that for the very large systems. However, as far as dilatancy is concerned, the $N = 98$ system displays negative shear dilatancy characteristic of the smaller systems.

Our new results for extremely large systems suggest that for low Reynolds number flows in two dimensions, the viscosity is independent of both system size and strain rate and that at constant N, V, T such a fluid is always *positively* dilatant.

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References

- [1] K. Kawasaki, and J.D. Gunton, "Theory of Nonlinear Transport Processes; Nonlinear Shear Viscosity and normal Stress Effects", *Phys. Rev. A*, **8**, 2048 (1973).
T. Yamada and K. Kawasaki, *Contributions of Statistical Mechanics far from Equilibrium IV*, Prog. Theo. Phys., **53**, 1111 (1975).
Y. Pomeau and P. Resibois, *Phys. Rept.*, **19**, 63 (1975).
J.P. Hansen and I.R. McDonald, *Theory of Simple Liquids*, p330 (Academic Press, London 1986).
- [2] D.J. Evans, "Nonlinear Viscous Flow in Two Dimensional Systems", *Phys. Rev. A*, **22**, 290 (1980).
- [3] D.J. Evans and G.P. Morriss, "Nonequilibrium Molecular Dynamics Simulation of Couette Flow in Two Dimensional Fluids", *Phys. Rev. Letts.*, **51**, 1776 (1983).
D.J. Evans and G.P. Morriss, "Shear Thickening and Turbulence in Simple Fluids", *Phys. Rev. Letts.*, **56**, 2172 (1986).
- [4] D.J. Evans and G.P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids*, p. 80 and p. 100. (Academic Press, London 1990).