

LETTERS TO THE EDITOR

The Letters to the Editor section is divided into three categories entitled Notes, Comments, and Errata. Letters to the Editor are limited to one and three-fourths journal pages as described in the Announcement in the 1 July 2001 issue.

ERRATA

Erratum: "Comparison of planar shear flow and planar elongational flow for systems of small molecules" [J. Chem. Phys. 113, 9122 (2000)]

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The expression given for the molecular pressure tensor [Eq. (12)] in the above paper contains a typographical error that unfortunately was not noticed in the original manuscript. This error may lead to some uncertainty regarding our computations. Equation (12) of the original paper currently reads

$$P_M V = \sum_{i=1}^N \frac{\mathbf{p}_i \mathbf{p}_i}{M_i} - \frac{1}{2} \sum_{i=1}^N \sum_{\alpha} \sum_{j \neq i} \sum_{\beta=1}^n \mathbf{r}_{i\alpha j\beta} \mathbf{F}_{i\alpha j\beta}^{\text{inter}}. \quad (1)$$

It should read

$$P_M V = \sum_{i=1}^N \frac{\mathbf{p}_i \mathbf{p}_i}{M_i} - \frac{1}{2} \sum_{i=1}^N \sum_{\alpha} \sum_{j \neq i} \sum_{\beta=1}^n \mathbf{r}_{ij} \mathbf{F}_{i\alpha j\beta}^{\text{inter}}, \quad (2)$$

where \mathbf{r}_{ij} is the minimum image separation of the centers of mass of molecules i and j . The correct expression was used in all computations. Equation (11) is correct for monatomic systems.

We note that the atomic pressure tensor for a molecular fluid should include all forces on a given atom, including constraint forces and other intramolecular forces. The averages of the molecular and atomic pressure tensors for molecular fluids are expected to agree in a shearing steady state. This expectation was always confirmed by our computations on small molecules. For larger molecules, which are capable of spanning the simulation box, it is possible for a site on a molecule to interact with another site on a different image of that molecule (imagine a molecule that is stretched out and inclined at a small angle to the horizontal). In this case, the expression for the molecular pressure tensor, Eq. (2), should include not only intermolecular force terms, but also forces between sites on different periodic images of the same molecule. A more detailed discussion of this point will appear in a paper that is currently in preparation.