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ON THE VISCOSITY OF A MODEL FLUID

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Abstract: N hard disks are injected into a 2-dimensional virtual pipe. The initial positions of the disks are generated according to the uniform distribution and the initial velocities according to a centered normal distribution. The Newtonian dynamics is imposed on the system (fluid) entailing a viscous fluid flow through the pipe. Since the flow velocity profiles can be assessed statistically during the computational process imitating the motion of the disks, computer experimental data carrying information about the dependence of viscosity on the thermodynamic conditions of the virtual fluid can be sampled. The statistical evaluation of these data leads to the establishment of a formula for the viscosity of the hard disk fluid. As an application, a possibility of the quantitative prediction of laboratory measurements of the viscosity of water as function of temperature is discussed.

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1. Introduction

If adjacent layers of a fluid move with different velocities, then a frictional force is acting on them. The material specific property enabling us to quantify the

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friction is viscosity which is also essential for predicting characteristics of fluid flow like Reynolds number, turbulence and drag coefficient.

In statistical physics there are some attempts to express the viscosity of a fluid as a function of variables that describe the thermodynamic state (density, temperature) and the microscopic properties of the constituents of the fluid.

From the kinetic theory of dilute gases the following formula for viscosity η of the hard sphere gas is obtained (cf. Reif [6], Section 12.3):

$$\eta = \gamma \cdot \frac{(m \cdot k_B \cdot T)^{1/2}}{r^2}, \tag{1.1}$$

where m and r denote the mass and the radius of the hard sphere, respectively, k_B is the Boltzmann constant and T the temperature; γ denotes a mathematical constant.

(1.1) suggests that viscosity of a gas does not depend on its density in the dilute range which is also confirmed by measurements. For liquids and dense gases, however, a correction of (1.1) is required because there is evidence for the dependence of viscosity on fluid density. The evidence stems from laboratory measurements (cf. Landolt, Börnstein [3]), from fluid mechanical considerations (cf. Vasudevaiah, Rajagopal [9]) and from molecular simulations (cf. Ishiwata et al [2])).

In the present contribution a computer experiment imitating the motion of the micro-constituents of a fluid is described which has been designed, implemented, carried out and statistically evaluated in order to study the dependence of viscosity of the hard disk fluid on its density.

Some important details of the molecular dynamics are presented in Section 2. Nonparametric kernel methods for the evaluation of the experiment are described in Section 3. The outcome of the long term computer experiment is reported in Section 4 where also a formula for the viscosity of the hard disk fluid is proposed. In Section 5 a resulting possibility of microscopic explanation of water viscosity in the temperature range $20°C - 100°C$ is presented.

2. The Dynamics of the Fluid

Let us consider a 2-dimensional pipe Π of radius b and length L:

$$\Pi = [0, L] \times [-b, b].$$

Initially the pipe is filled with a fluid consisting of N hard disks of mass m and radius r. The initial positions of the disks are generated according to the uniform distribution on Π subject to the condition of mutual non-overlapping.

The initial velocities of the disks are generated according to the 2-dimensional normal distribution

$$N(0, \sigma^2) \otimes N(0, \sigma^2) \tag{2.1}$$

with the thermodynamic interpretation of the variance

$$\sigma^2 = \frac{k_B \cdot T}{m}, \tag{2.2}$$

where T denotes the temperature of the system. This initial microstate complies with Maxwell hypothesis (cf. Moeschlin, Grycko [4], Chapter 1).

Newtonian dynamics is imposed on the system (for conceptual and algorithmic details cf. Moeschlin, Grycko [4]). The outcomes of collisions between disks are determined by the laws of momentum and energy conservation.

If a disk arrives at the left boundary $\{0\} \times [-b, b]$ of the pipe, then it is simply reflected. If a disk arrives at the right boundary $\{L\} \times [-b, b]$, then it is injected close to the left boundary and its velocty is generated according to (2.1). If a disk arrives at the lower or at the upper boundary of Π (at $[0, L] \times \{-b\}$ or at $[0, L] \times \{b\}$), then its velocity is generated according to (2.1) subject to the condition that the velocity vector points to the interior of Π; this kind of reflection is called isothermal nonslip condition (cf. Ishiwata et al [2]).

The described dynamics entails that the fluid consisting of N hard disks starts flowing through the pipe. According to our experience, after some time the fluid flow becomes stationary and the temperature stabilizes itself at a value which is significantly lower than the temperature corresponding to the variance in (2.1).

A basic notion describing fluid flow in the continuum picture is the velocity field $u : \Pi \to \mathbb{R}^2$ known from fluid mechanics (cf. Chorin, Marsden [1]); the vector $u(x_1, x_2)$ is interpreted as the velocity of the fluid at $(x_1, x_2) \in \Pi$. A bridge between the atomistic and continuum pictures is provided by the Nadaraja-Watson regression estimator which is presented in Section 3.

From fluid mechanics it is known (cf. Tritton [8]) that the the first component u_1 of the velocity field of a fluid flow through a pipe is given by

$$u_1(x_1, x_2) = \frac{-\partial p / \partial x_1}{2 \cdot \eta} \cdot (b^2 - x_2^2), \tag{2.3}$$

where $\partial p / \partial x_1$ denotes the pressure gradient w.r.t the horizontal coordinate x_1 and η denotes the viscosity of the fluid. Since $u_2 = 0$, (2.3) indicates that the velocity profiles at vertical sections through the pipe are parabolas whose parameters depend in particular on the viscosity η of the fluid, which is utilized for estimation of η from computer experimental data.

3. The Statistical Tools

The microscopic state of a fluid consisting of N micro-constituents at time $t \geq 0$ is described by the $4N$-tuple

$$(x^{(1)}(t), \ldots, x^{(N)}(t), v^{(1)}(t), \ldots, v^{(N)}(t)) \in \Pi^N \times \mathbb{R}^{2N}, \tag{3.1}$$

where $x^{(j)}(t)$ denotes the momentary position and $v^{(j)}(t)$ the momentary velocity of the j-th micro-constituent.

Let $K : \mathbb{R} \to \mathbb{R}_+$ be the Gaussian kernel

$$K(x) := (2\pi)^{-1/2} \cdot \exp(-\frac{1}{2}x^2).$$

Let $\varrho : \Pi \to \mathbb{R}_+$ be the particle density of the fluid at a fixed time $t \geq 0$ understood as a function of the space coordinates (x_1, x_2). Under the model assumption that ϱ is constant on vertical cuts $\{x_1\} \times [-b, b]$ through the pipe, $0 \leq x_1 \leq L$, ϱ can be estimated by the kernel density estimator

$$\widehat{\varrho}(x_1, x_2) := \frac{1}{2bh} \sum_{j=1}^{N} K\left(\frac{x_1 - x_1^{(j)}(t)}{h}\right), \tag{3.2}$$

where $h > 0$ denotes an appropriate bandwidth and $x_1^{(j)}(t)$ the horizontal coordinate of the position vector $x^{(j)}(t) \in \Pi$. A natural estimator of the gradient $\partial\varrho/\partial x_1$ of the particle density function is given by the derivative $\partial\widehat{\varrho}/\partial x_1$ of $\widehat{\varrho}$. The application of estimators $\widehat{\varrho}$ and $\partial\widehat{\varrho}/\partial x_1$ is motivated by consistency results, cf. Nadaraya [5].

In order to estimate the pressure gradient, we utilize the equation of state

$$p = k_B \cdot T \cdot (\varrho + \sum_{i=1}^{6} A_i \cdot (2\sqrt{3}r^2)^i \cdot \varrho^{i+1}) \tag{3.3}$$

for hard disk fluid where the virial coefficients $A_1, \ldots, A_6$ are approximated according to Wang et al [10]. A natural estimator $\widehat{G}$ of pressure gradient $G := \partial p/\partial x_1$ is given by

$$\widehat{G} = k_B \cdot \widehat{T} \cdot \left(1 + \sum_{i=1}^{6} (i+1) \cdot A_i \cdot (2\sqrt{3}r^2 \cdot \widehat{\varrho})^i\right) \cdot \frac{\partial\widehat{\varrho}}{\partial x_1}, \tag{3.4}$$

where the temperature estimator $\widehat{T}$ is defined according to

$$\widehat{T} := \frac{m \cdot \sum\limits_{j=1}^{N} (v_2^{(j)}(t))^2}{k_B \cdot N}. \tag{3.5}$$

Let the momentary state (3.1) be interpreted as a realization of a tuple

$$(X^{(1)}, \ldots, X^{(N)}, V^{(1)}, \ldots, V^{(N)})$$

of random vectors. The velocity field $u : \Pi \to \mathbb{R}^2$ known from fluid mechanics (cf. Chorin, Marsden [1]), is now interpreted as the conditional expectation of the velocity vector V of a micro-constituent w.r.t its position vector X:

$$u(x_1, x_2) = E(V | X = (x_1, x_2))\,. \tag{3.6}$$

The Nadaraja-Watson estimator $\widehat{u}$ of u based on the momentary state (3.1) is given by

$$\widehat{u}(x_1, x_2) = \frac{\sum\limits_{j=1}^{N} v^{(j)}(t) \cdot K\left(\frac{x_1 - x_1^{(j)}(t)}{h}\right) \cdot K\left(\frac{x_2 - x_2^{(j)}(t)}{h}\right)}{\sum\limits_{j=1}^{N} K\left(\frac{x_1 - x_1^{(j)}(t)}{h}\right) \cdot K\left(\frac{x_2 - x_2^{(j)}(t)}{h}\right)}\,, \tag{3.7}$$

where $h > 0$ is a bandwidth. This application of the Nadaraja-Watson estimator is motivated by consistency results from Schuster, Yakowitz [7].

Let us fix a vertical cut $\{x_1\} \times [-b, b]$ through the pipe. In view of (3.7), an estimator of the velocity profile $(u_1(x_1, x_2))_{x_2 \in [-b,b]}$ is given by

$$(\widehat{u}_1(x_1, x_2))_{x_2 \in [-b,b]}; \tag{3.8}$$

therefore the value of parameter ξ of the parabola $(\xi(b^2 - x_2^2), x_2)_{x_2 \in [-b,b]}$ can be fitted to the nonparametric estimate (3.8) of the velocity profile by the least squares method yielding an estimator $\widehat{\xi}$ of parameter ξ. In view of (2.3) an estimator $\widehat{\eta}$ of viscosity η of the fluid at the cut $(x_1, x_2)_{x_2 \in [-b,b]}$ is given by:

$$\widehat{\eta} = \frac{-\widehat{G}}{2 \cdot \widehat{\xi}}\,. \tag{3.9}$$

All estimators considered in this section are based on computer experimental data (3.1) describing a momentary microstate of our model fluid flowing through pipe Π. Therefore we are able to estimate the thermodynamic parameters (cf. (3.2) and (3.5)) and the viscosity of the fluid at an arbitrary time point $t > 0$ and at an arbitrary cut $(x_1, x_2)_{x_2 \in [-b,b]}$ through the pipe. The appropriateness of estimator $\widehat{\eta}$ of viscosity is based on the assumption of parabolicity of the velocity profiles which is justified by basic considerations in fluid mechanics (cf. Tritton [8]). This assumption is also confirmed by graphical comparison between parametric and nonparametric estimates of the velocity profiles (cf. Section 4).

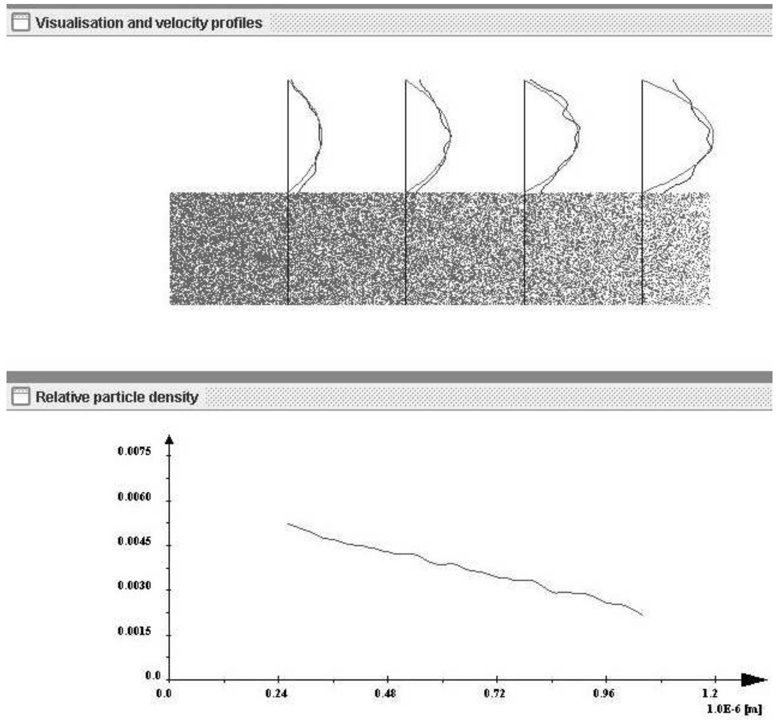

Figure 1: Screen shot of the computer experiment

4. The Computer Experiments and their Evaluation

In all computer experiments $N = 8 \cdot 10^4$ hard disks of radius $r = 1\text{Å} = 10^{-10}\text{m}$ and mass $m = N_A^{-1}$ has been injected into the pipe according to Section 2 ($N_A = 6.02 \cdot 10^{26}\text{kg}^{-1}$ denotes the modified Avogadro number). The parameters L and b of pipe Π are implicitely defined by

$$L = 16b \qquad \text{and} \qquad \frac{N}{2bL} = \frac{\varrho_r}{2\sqrt{3} \cdot r^2}\,, \tag{4.1}$$

where the initial relative density ϱ_r has been varied within the range 10^{-3}–10^{-2}. Then Newtonian dynamics has been imposed on the micro-constituents of the fluid under inclusion of an isothermal nonslip condition (cf. Section 2). The initial temperature has been set to $T = 300\text{K}$.

Figure 1 shows a screen shot of an experiment after 702000 collisions where the initial relative density has been set to $\varrho_r = 1/400$. In the upper window the pipe filled with the fluid is shown. At four cuts through the pipe the nonparametric and the parametric estimates of the velocity profiles are visualized; since corresponding estimates are close to each other, the screen shot confirms the parabolicity of the velocity profiles which complies with the predictions from fluid mechanics, cf. Tritton [8]. In the lower window of the screen shot, an estimate of the relative density of the fluid as function of the horizontal space coordinate x_1 based on the estimator

$$\widehat{\varrho}_r(x_1, x_2) = 2\sqrt{3}r^2 \cdot \widehat{\varrho}(x_1, x_2) \tag{4.2}$$

(cf. (3.2)) is graphed; the estimate shows a decreasing fluid density along the flow as expected.

The evaluation of the computer experiments is based on the ansatz

$$\eta = \gamma(\varrho_r) \cdot \frac{(m \cdot k_B \cdot T)^{1/2}}{r} \tag{4.3}$$

for the viscosity η of the hard disk fluid. (4.3) can be viewed as the 2-dimensional pendent of (1.1) with the modification that factor γ may depend on the relative density of the fluid.

At a particular time point of an experiment the data (3.1) describing the microstate of the fluid are available; 100 equidistant cuts $\{x_1\} \times [-b, b]$ through the pipe are considered, where $L/4 \leq x_1 \leq 3L/4$. At every cut the relative density and the viscosity can be estimated (cf. (4.2) and (3.9)); an estimator of temperature T is given in (3.5); based on these estimators and on (4.3) we are able to sample 100 pairs $(\widehat{\varrho}_{ri}, \widehat{\gamma}_i), i = 1, \ldots, 100$, carrying statistical information about the dependence of factor γ in (4.3) on the relative density.

The whole procedure is repeated at appropriate time points yielding a large data set consisting of blocks of length 100.

Analogous experiments have been carried out where the initial relative density ϱ_r has been set equal to 1/700, 1/600, 1/400, 1/250, 1/150 and to 1/100 requiring a total of about one year of processor time.

Figure 2 shows a diagram, where the abscissas correspond to the estimates of relative density ϱ_r and the ordinates to the estimates of parameter γ. The cloud reveals a strong dispersion of the estimators. The continuous line in the diagram shows the Nadaraya-Watson estimate of the functional dependence between the estimated parameters. The Nadaraya-Watson estimate suggests that there is a monotonic dependence of γ on ϱ_r which can be detected only if a very large number of data points are involved. The visual impression motivates the ansatz

$$\gamma(\varrho_r) = \exp(\alpha \cdot \varrho_r + \beta) \tag{4.4}$$

for the dependence of parameter γ on the relative density, where the constants

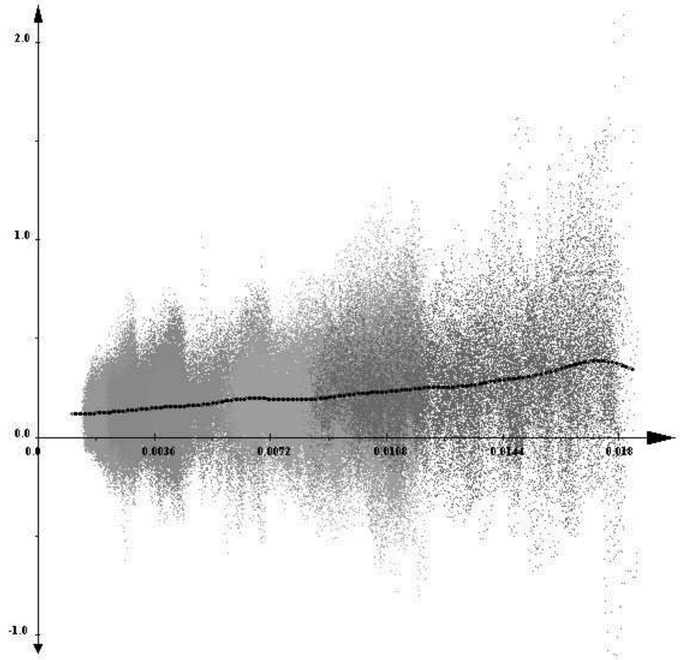

Figure 2: Estimates of γ versus estimates of relative density

α and β can be fitted to the (nonparametric) Nadaraya-Watson estimate.

The least-squares method yields

$$\widehat{\alpha} = 52.71 \qquad \text{and} \qquad \widehat{\beta} = -2.06.$$

Summarizing we claim that based on our computer experimental experience the formula

$$\eta = \exp(\widehat{\alpha} \cdot \varrho_r + \widehat{\beta}) \cdot \frac{(m \cdot k_B \cdot T)^{1/2}}{r} \tag{4.5}$$

for the viscosity η of the hard disk fluid is approximatively valid in the range $0.001 < \varrho_r < 0.02$ of relative density ϱ_r.

5. The Viscosity of Water

Since the viscosity of water as function of temperature can be measured in laboratory, a challenging question is whether the decrease of water viscosity with increasing temperature can be explained by the 3-dimensional pendant of

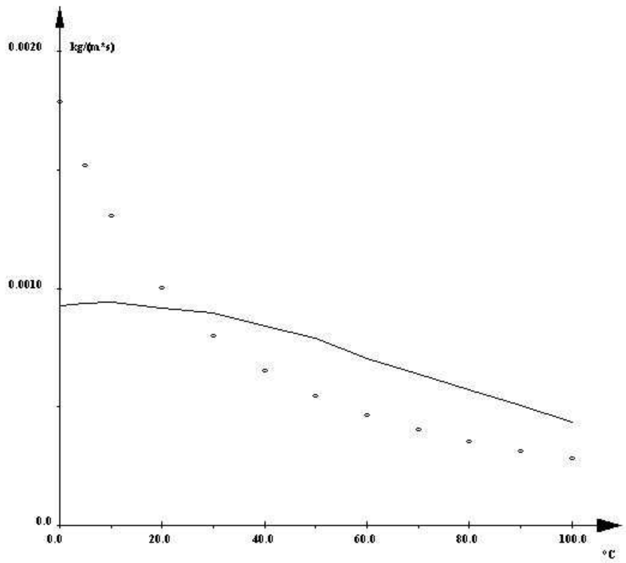

Figure 3: Viscosity of water as function of temperature

the microscopically justified formula (4.5):

$$\eta = \exp(\alpha \cdot \varrho_r + \beta) \cdot \frac{(m \cdot \ k_B \cdot T)^{1/2}}{r^2}. \tag{5.1}$$

In Figure 3 the laboratory measurements of water viscosity in the temperature range $0°C - 100°C$ are shown. The continuous line corresponds to the prediction (5.1), where the parameters α, β and r have been fitted to the measurements by the least-squares method yielding

$$\widehat{\alpha} = 91.59, \qquad \widehat{\beta} = -26.60 \qquad \text{and} \qquad \widehat{r} = 1.157 \cdot 10^{-10}\text{m}.$$

Figure 3 confirms the approximative validity of (5.1) for water viscosity in the temperature range $20°C - 100°C$ entailing a realistic value $\widehat{r}$ of the molecular radius; the discrepancy between (5.1) and laboratory measurements in the range $0°C - 20°C$ can be interpreted as a limitation of the hard disk model in the context of microscopic explanation of viscosity of water.

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