Fluctuation-dissipation theorems and transport coefficients of the gases, liquids and nanofluids

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Abstract. In present paper a problem of the determination and calculation of transport coefficients is discussed. Gases, liquids, dispersed fluid including nanofluids are considered. The special section deals with the transport processes in fluids under confined conditions. The fluctuation dissipation theorems for transport coefficients of the turbulent fluid are formulated. It was shown that in all cases the transport coefficients are determined by the fluctuation-dissipation theorems. In according with these theorems the transport coefficients are the integrals of the correlation functions of the microfluctuations of the corresponding dynamical variables. The structure of the viscosity coefficient of all media mentioned above is analysed in detail. In the last part of the paper these viscosity coefficients are calculated by the molecular dynamics method.

1. Introduction

The modern understanding of the objects around us is based on their molecular structure. The idea of describing the substances properties from the first principles, based on their molecular structure, goes back to the classic works of Maxwell and Boltzmann. In such way it was possible to describe the dynamics of the rarefied gas and the corresponding transport processes (see, for example, [1]). An attempt to generalize the Boltzmann approach for dense gas was made by Enskog [1]. He derived the kinetic equation for the dense gas of hard spheres. In the Enskog’s gas, there are only binary collisions of molecules, as in a rarefied gas. Therefore the Enskog equation has the same structure as the Boltzmann one. There is only one difference. In the Boltzmann equation molecules are material points, whereas in the Enskog equation they have finite sizes. However, the multiparticle collisions of molecules (triple, etc.) are possible in a dense gas. Is it possible to construct a transport theory from the first principles in such systems?

The answer to this question was given in the famous monograph of Bogolyubov [2]. Before this answer is formulated, it should be noted that the dynamics of disordered molecular systems (gases and liquids) can be described on three different levels [3]. The most detailed, microscopic, requires knowledge of all the dynamic variables of the system (coordinates and velocities). To implement this description, it is necessary to solve the corresponding system of the Newton equations or the equivalent Liouville equation for the \( N \)-particle distribution function \( F_N \). The next, much less detailed level of description is the kinetic one. In this case the kinetic equation for a single-particle distribution function \( F_1 \) is formulated (the kinetic Boltzmann theory corresponds namely this level of description). Finally, the macroscopic level of description by means of macroscopic variables \( \phi_A \) (density, velocity, temperature, etc.) is the least detailed and usually used in practice.
Bogolyubov put forward the idea of reducing the level of description. He proposed to search for a class of solutions of the BBGKI-hierarchy of kinetic equations, in which the evolution of s-particle distribution functions is consistent with the change in time of one-particle one. The macroscopic level is possible if the dependence on the time of the one-particle function is determined by the evolution of macroscopic variables. The fruitfulness of this idea was shown by the example of a moderately dense gas [4]. However, it is clear that in higher density approximations this approach is not applicable, here the kinetic description is simply impossible. In a dense system, calculating even energy at equilibrium state requires at least a pair distribution function. In principle, this problem was solved in [5] using the boundary condition of partial weakening of initial correlations. But the resulting kinetic equations are extremely complex and cannot be solved in principle. In addition, it is clear that the resulting series in density, generally speaking, do not converge.

On the other hand, the construction of a kinetic description of condensed media is not usually required. As a rule, dynamics of condensed medium may be described by the transport equations (hydrodynamic equations). In this case, a fundamental problem arises of determining the transport coefficients. The only way to solve this problem is their molecular modeling, which should also be based on first principles. Present work is devoted to the description of the procedure for determining the transport coefficients and their molecular modeling. The transport processes in different systems (gas, liquid, nanofluids, fluid under confined conditions) are considered and analyzed.

2. Statistical mechanics of the transport processes in condensed media

One of the main problems of the transport theory of condensed media is the derivation of the constitutive relations. The complexity of solving this problem is due to the fact that these relations depend on the dynamics of all the particles of the system under consideration. There are two ways to solve this problem. On the one hand, we can try to directly solve the Newton's equations describing the dynamics of the system. This approach is implemented in the molecular dynamics (MD) method. However, in this case only the dynamic variables of the system, the coordinates and velocities of all its particles, are obtained. We need a regular method of calculating with the help of these variables all observables: density, pressure, temperature, etc. To this end, it is necessary to use the methods of nonequilibrium statistical mechanics. In fact, all observables are calculated using the $N$-particle distribution function. This function is a solution of the Liouville equation

$$\frac{\partial F_N}{\partial t} = \sum_{i=1}^{N} \left( \frac{\partial H_N}{\partial r_i} \cdot p_i + \frac{\partial H_N}{\partial p_i} \cdot r_i \right) = 0,$$  \hspace{1cm} (1)

where $r_i$ and $p_i$ are the coordinate and impulse of the particle $i$ and $H_N$ is the Hamiltonian of the system. To describe the transport processes in the system considered we have to construct the solution of equation (1) corresponding to the macroscopic level of the system description. Such solution can be constructed by use of the projection method [6]. There are many different variants of this method [7-10]. However in all cases the similar generalized constitutive relations are obtained. These relations for the isotropic medium have the following form

$$J_i(r,t) = J_i(r,0) + \int_0^t \int d\tau K_{ni}(r,r',\tau-t) \cdot X_n(r',t), \hspace{1cm} i = 1,2,3.$$  \hspace{1cm} (2)

Here $X_n$ are so-called thermodynamical forces. These forces are equal to the gradients of the macroscopic variables. The constitutive relations (2) are nonlinear, nonlocal and delaying. The nonlinearity of the relations (2) is due to that the transport kernels $K_{ni}$ are also the functionals of the thermodynamical forces. The delay is connected with the finite speed of propagation of disturbances in the medium. The spatial nonlocality is associated with the correlation between dissipative fluxes $J_i$ and thermodynamic forces and is due to the nonlocality of the particles interactions and statistical effects (interactions of the physical small fluid volumes).

In this paper we will consider the weakly nonequilibrium processes. In this case the dissipative fluxes are proportional to gradients of the macroscopic variables $\varphi_i$. 

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\[ J_i(r, t) = -\mu_i \nabla \Phi_i(r, t), \quad i = 1, 2, 3. \quad (3) \]

The transport coefficients in linear constitutive equations (3) are the integrals over the time from the two-time correlation functions \( \chi_i \) of the corresponding dynamical variables

\[ \mu_i = \int_0^t dt_1 \chi_i(r, t - t_1), \quad i = 1, 2, 3. \quad (4) \]

These relations are named as fluctuation-dissipation theorems (FDT). In literature for the simple fluids these theorems are known as Green-Kubo formulas [8, 10, 11].

It would like to note two important facts. The transport coefficients of the weakly nonequilibrium fluid flows are determined by the microfluctuations of the corresponding dynamical values. The correlation functions in equation (4) are calculated by means of equilibrium distribution function. Thus the transport coefficients (4) are the properties of equilibrium state of the system.

3. Universality of the fluctuation-dissipation theorems

The simplest FDT determines the self-diffusion coefficient

\[ D = \frac{1}{3} \int_0^{t_p} dt_1 \chi_1(r, t - t_1). \quad (5) \]

The coefficient (5) is the function of the time. This dependency is determined by the evolution of the velocity autocorrelation function (VACF)

\[ \chi_1(t) = \sum_{i=1}^N \langle v_i(0) \cdot v_i(t) \rangle. \quad (6) \]

Here angle brackets indicate ensemble averaging. Thus VACF as all other correlation functions is calculated using the \( N \)-particle distribution function. The observed value of this coefficient is obtained when it reaches a plateau value \( t_p \) [12]. Therefore the existence of transport coefficients means that the corresponding correlation function must be decaying. Really, VACF of the rarefied gas damps exponentially [13, 14]. The evolution of VACF of the dense gas is more complex, it has two different branches

\[ \chi_1(t) = a e^{-\frac{t}{\tau}} + b(t - t_*)^{-\frac{3}{2}}. \quad (7) \]

Here \( a, b \) and \( t_* \) are some constants. The character of the VACF decay determines the mechanism of the particles diffusion in a medium.

3.1. Viscosity of the nanofluid

A nanofluid represents a binary system consisting of a carrier fluid and nanoparticles. They are being used to advantage or are intended to be used in (i) new medicinal preparations and cosmetic products; (ii) biotechnology, nanotechnologies of different application; (iii) different thermophysical applications; (iv) drug delivery systems; (v) different contamination detectors, water cleanup systems, and air cleaning units; and (vi) new lubricants, lacquers, paints, and construction materials. In all these applications we have the flows of the nanofluids. Therefore the viscosity of nanofluids is very important their characteristics. Today it has been established that the viscosity of nanofluids does not described by the classical theories [15, 16]. FDT of the viscosity of the nanofluid has the following form

\[ \eta = \frac{1}{5kT} \int_0^{t_p} dt \langle J(0); J(t) \rangle, \quad (8) \]

where \( J \) is the microscopic formula of the stress tensor

\[ J = \sum^2_{\alpha} \sum_{i=1}^{N_{\alpha}} \left[ m_{\alpha} v_i v_i + \frac{1}{2} \sum_{\alpha, i \neq j} (r_i - r_j) F_{ij} \right], \quad (9) \]
here $r_i$ and $v_i$ are the coordinate and velocity of the particle $i$ of phase $\alpha$, $m_\alpha$ is its mass and $F_{ij}$ is interparticle force. $T$ is the fluid temperature, $k$ is the Boltzmann constant. Here indices $\alpha = 1, 2$ refer to base fluid molecules and nanoparticles, respectively.

3.2. Viscosity of the fluid in confined conditions

Extensive study of fluid flows under confined conditions in the last years has been motivated by the traditional interest to the flows in porous media on the one hand, and by emergence of many different microfluidics tools and systems on the other. Such microflows are currently use in biochemistry, medicine, pharmacology, biology, thermal engineering, catalysis, etc. An important aspect of the active use of various micro and nanoflows is the development of a new generation of resource-saving technologies with low power consumption. The efficiency of micro and nanodevices is largely determined by the transport processes occurring in the fluid flows. Thus, for example, the energy spent for fluid circulation depends on the fluid viscosity. Today, however, it is known that transport processes in confined conditions are significantly different from those in the bulk. In papers [17, 18] the statistical mechanics of the fluid transport properties under confined conditions were developed. The considered system (fluid molecules and atoms of the walls of channel or pores) is modelled by the two kinds of the particles. The evolution this particles system is described by equation (1). Solving this equation, the constitutive relations were derived. It has been established that the transport properties of fluids in nanochannels and nanopores are determined not only by the characteristics of the fluid, but also by the properties of the entire fluid-channel (pore) wall system. In particular, the effective viscosity coefficient of the fluid is described by the following FDT

$$\eta = \frac{1}{5kT} \sum_{i,j=f,b,i\neq j}^{t_p} \int dt \left( J_f(0):J_f(t) + J_i(0):J_{ij}(t) \right). \quad (10)$$

Here the subscript $f$ corresponds to the fluid molecules, and $b$ to the molecules (atoms) of the channel walls. In addition, new type stress tensor of the the microscopic fluxes is appeared

$$J_{fb} = -\frac{1}{4} \sum_{\alpha}^{N_\alpha} \sum_{i}^{2} (r_i - r_j) F_{ij}. \quad (11)$$

The equations (10), (11) are the generalization of the known Green–Kubo formula for the fluid in the bulk (the last obtains from equations (8), (9) for $\alpha = 1$). The effective viscosity coefficient due to the interactions not only between the fluid molecules. The interactions of the fluid molecules with the walls play a key role also. This should be taken into account, and it should be realized that the fluid viscosity in nanochannels is not determined only by the fluid properties. This system is a special two-phase medium in which transport processes are in a sense similar to those in two-phase suspensions, where it is also necessary to introduce effective transport coefficients.

3.3. Fluctuation-dissipation theorems for the turbulent fluid flows

The FDTs are the fundamental relations of the theory of dissipative processes. In all cases when we may introduce the transport coefficients describing given dissipative process these coefficients will be integrals from two-time correlation functions of appropriate microfluctuationes. In particular, we may consider the transport processes in turbulent fluid flows. In turbulent flows the instant velocity field $u$ may be presented as superposition of the average velocity $U$ and fluctuation $\delta u$: $u = U + \delta u$. In simplest case the turbulent dissipative processes will be determined namely these fluctuations. Therefore it is possible to introduce the coefficient of turbulent diffusion

$$D_t = \frac{1}{3} \int dt \left( \delta u(0) \cdot \delta u(t) \right). \quad (12)$$

Further, the similar way we may determine the turbulent viscosity coefficient
\[
\eta_t = \frac{1}{5kT} \int_0^{t_p} dt \langle \delta u(0) \delta u(t) \rangle,
\]
(13)

coefficient of the transfer of the turbulent energy

\[
\lambda_t = \frac{1}{3} \int_0^{t_p} dt \langle \delta u^2(0) \delta u(0) \cdot \delta u^2(t) \delta u(t) \rangle,
\]
(14)

and coefficient of thermal diffusion

\[
D_{et} = \frac{1}{3} \int_0^{t_p} dt \langle \delta u^2(0) \delta u(0) \cdot \delta u(t) \rangle.
\]
(15)

Certainty, in general case the transport processes in turbulent flow are rather complex. Therefore the formulas (12)–(15) will have more complicated form. We have to take into account the presence of the pressure and density fluctuations. In addition, all fluctuations will be interacted with each other. Finally, there are fluctuations of different scales. For this reason it will be convenient to formulate the corresponding transport coefficient in Fourier representation. However all FDT will have the form similar to the formulas (12)–(15).

4. Molecular dynamics simulation of the viscosity coefficient

We wrote above that the correlation functions and consequently transport coefficients are calculated by means of \(N\)-particle distribution function. Therefore it is possible to calculate transport coefficients analytically in simplest case of the rarefied gas only. In all other cases a single way to get the corresponding information is the molecular dynamic (MD) method. MD simulation of the viscosity coefficients (8) and (10) is the subject of this section.

The standard molecular dynamics method is employed (see e.g., [19]). We used the standard free package LAMMPS and original SibMD package that was applied earlier for solving various problems of transport processes of nanofluids (see papers [20-22] and references therein). The simulation was carried out in a cubic cell with periodic boundary conditions. The interaction of molecules of the carrier medium was determined by the Lennard-Jones potential. The interaction of molecules of the carrier medium with a nanoparticle was determined by the special derived potentials [23, 24]. Verlet scheme was used to integrate the Newton equations. NVE and NVT thermostats were used. The integration step was equal to one femtosecond.

Since the phase trajectories of the system are locally unstable and mixed in the molecular dynamic calculation [14, 25], the obtained results must be averaged over the ensemble of independent phase trajectories. In this study, averaging was carried out over 1000 (up to 10000) independent phase trajectories.

4.1. Simulation of the viscosity coefficient of the water

Water is known to be an extremely complex fluid. A lot of special intermolecular potentials have been developed early to describe its various properties and to simulate them by the molecular dynamics method [26–29]. These potentials are multiparameetric, it is not easy to determine reliably these parameters. As a result, the transport properties of water have not yet been able to be simulated accurately enough (at least with the accuracy of the corresponding experimental measurements), despite the fact that such attempts are made continuously (see, [30–32] and references therein). The viscosity coefficient is the integral properties of the water therefore we are sure that may use the simple Lennard-Jones potential.

Calculation of correlation functions was carried out on time equal to \(\tau = 20\) picoseconds. Figure 1 shows the evolution of the viscosity correlation function normalized by its initial value (a) and viscosity coefficient (b) for 64 thousand molecules in a simulation cell as an example. The viscosity coefficient (4) reaches the plateau value in 3–5 picoseconds.
Figure 1. Time dependences of the normalized stress tensor correlation function of water (a) and the viscosity coefficient (b). Time is measured in picoseconds, viscosity coefficient in Pa·s·10^4.

The simulation accuracy increases with the number of molecules. In the presented data, the number of molecules $N$ was varied from 4000 to 64000. The simulation accuracy was determined by the comparison of the calculated and experimental [33] data. The simulation accuracy increases monotonically with an increase in the number of particles, and the relative error $\Delta \sim 1/\sqrt{N}$. Using 64000 molecules, we obtain the accuracy of the order of the experimental one.

4.2. Simulation of the viscosity coefficient of the water-based nanofluids

This section contains the discussion of the results of simulating the viscosity of a water-based nanofluid with copper particles. The diameter of the nanoparticle is equal to 2, 4, and 10 nanometers. The number of molecules and nanoparticles was largely determined by the mass density of water under normal conditions and by the volume fraction of nanoparticles and their sizes. The number of nanoparticles was ranged from 8 to 64, and the number of molecules was varied from seventy thousand to a half of million.

Figure 2. Dependence of the relative viscosity coefficient of the water-based nanofluids on the volume concentration of the Cu nanoparticles.

The obtained data are presented in figure 2, where the dependence of the relative viscosity coefficient $\eta_r = \eta/\eta_0$ on the volume fraction of nanoparticles $\phi$ ($\eta_0$ is the viscosity coefficient of water) is shown. Here, round labels and dash-dotted line correspond to nanofluid with 2 nanometer particles, triangles and a dotted line correspond to 4 nanometers particles, and a square label corresponds to 10 nanometers particle. Dashed line corresponds to the Batchelor formula $\eta = \eta_0(1 + 2.5\phi + 6.2\phi^2)$ [34]. In all cases, the dependence of the viscosity coefficient on the concentration of nanoparticles is described by the following relation.
\[
\eta = \eta_0 (1 + a\varphi + b\varphi^2).
\]  
\(\text{(16)}\)

Comparison of the presented data shows that in all cases the viscosity coefficient is significantly higher than the coefficient, obtained by the Batchelor formula for coarse-grained dispersed liquids. Thus, the effective viscosity coefficient of nanofluid even at low concentrations of particles is not described by the classical theories of Einstein and Batchelor. The dependence is linear for small nanoparticles volume concentrations, and then the quadratic term in (16) begins to play significant role. As the diameter of the nanoparticles increases, the viscosity of the nanofluid decreases. This is consistent with the calculations for other nanofluids and experiments [15, 16].

4.3. Fluid viscosity in nanochannels
In section 3.2 is shown that FDT for viscosity coefficient of fluid under confined condition is described by the formulas (10), (11). The purpose of this section is to perform MD calculation of the viscosity of fluids in a plane nanochannel and study the factors that determine the fluid viscosity. The viscosity of benzene in channels of different heights is investigated.

All intermolecular interactions were described by the cutoff Lennard-Jones potential. The effective viscosity coefficient of a fluid in the nanochannel was compared with the viscosity coefficient of the same fluid in a bulk, which was also simulated by the MD method. The comparison was carried out at the same pressure and fluid temperature.

![Figure 3](image_url)

**Figure 3.** Viscosity coefficient versus channel height (in Angstroem units) for the following types of fluid and channel walls: C\textsubscript{6}H\textsubscript{6}-C (○), Ar-Ar (■), C\textsubscript{6}H\textsubscript{6}-Al (●).

The typical obtained result is presented in figure 3 [35], which shows curves of the normalized viscosity coefficient of benzene at room temperature versus height of channels \(h\) with different wall materials. The lines in the figure correspond to the approximations of the results by the function \(\eta_r = (1 \pm B/h)\) in which the constant \(B\) depends on the properties of the fluid and the walls. In the nanochannel with walls of carbon, whose molecules have a small value of \(\varepsilon\) (the depth of the potential well of Lennard-Jones potential), the viscosity of benzene decreases. On the other hand, there is an increase in viscosity in the channel with aluminum walls. It can be argued that it is the great depth of the potential well of aluminum molecules that leads to an appreciable increase in viscosity. In all cases, the differences between the viscosity coefficient in the nanochannel and the \(\eta_0\) value increase monotonically with decreasing channel height.

5. Conclusion
In conclusion we would like to note two circumstances. Fluctuation-dissipation theorems have universal character. They describe the transport properties as in one-phase also in two-phase fluids.
(gas and liquid). The existence of FDT indicates that the transport properties are determined by the evolution of microfluctuations of the dynamic variables of the given fluid. Therefore the transport coefficients of ordinary (Newtonian) fluids are their equilibrium properties. Situation with non-Newtonian fluids is more complicated. In ordinary sense we cannot speak about viscosity coefficient of such fluid. The measured viscosity of such fluid depends not only on their equilibrium properties but also on the shear velocity.

On the other hand, the situation with another transport coefficients are simpler. For example, the diffusion coefficient of the polymer solution can be calculated by means of FDT. The diffusion coefficient of dispersed particles (for example, nanoparticles) is determined by FDT also. The calculation of the thermal conductivity is more complicated. In this case it is necessary to exclude the energy transfer associated with diffusion.

In this article, the molecular dynamics simulation of the viscosity of a nanofluid based on water with copper particles is performed. This, in turn, required the determination of the viscosity of water with sufficiently high accuracy. The accuracy of the simulation should be comparable with the accuracy of the experimental measurement of the viscosity of water (usually 1–2%). This was achieved using a fairly simple potential for the interaction of molecules, the Lennard-Jones potential. Today we can say with confidence that the viscosity of nanofluids is significantly higher than the viscosity of ordinary coarse dispersed fluids. In contrast to the viscosity of coarse dispersed fluid the viscosity of nanofluids depend not only on the particle concentration but also on their size and material. The reasons of such behavior are clear. The main one is that the nanofluid is much more ordered (in the sense of short-range order) fluid than the base liquid [36].

This study has shown that the viscosity in nanochannel is largely determined by the walls of the channel. This is due to the fact that the momentum redistribution process in the system depends significantly on the interaction between the fluid molecules and the channel walls, and it is this process that determines the viscosity. The fluid viscosity in nanochannels is not determined only by the fluid properties. In this case, it is necessary to introduce the effective viscosity (and thermal conductivity) of the entire fluid–wall system.

Many experiments have demonstrated a significant reduction in flow resistance in microchannels [37, 38]. This was usually associated with the slip effect in such channels [39]. However, as indicated above, such a reduction in flow resistance may also be due to a decrease in the effective viscosity of the fluid compared to its viscosity in bulk.

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