

# TRANSPORT COEFFICIENTS OF A FLUID AT NANOSCALE

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**Summary** The Chapman-Enskog functional perturbation method is employed to solve the derived Enskog-like integro-differential kinetic equation which describes the dynamical behavior of a fluid at nanoscale. The analytical solutions for the nanofluid viscosity, thermal conductivity and other nominal transport coefficients are acquired according to the reduced transport equation and classical definitions in fluid mechanics. The molecular dynamics (MD) simulation is further used to verify the theoretical results via the model of a Lennard-Jones fluid in a nano Couette flow.

## INTRODUCTION

The present research aims at acquiring the transport coefficients of a nanofluid. To understand these dynamic properties is an important step to further explore nanofluid dynamics. It is assumed in this paper that a nanofluid is composed of a bulk of fluid molecules, and the dynamic structures and movements of molecules generate all the physical properties. Under such assumptions, the transport coefficients of a nanofluid may be obtained from the Boltzmann equations through which the particle-like molecular behaviors may well be depicted.

## KINETIC THEORY FOR NANOFLUIDS

As a nanofluid contains enormous number of atoms or molecules, its dynamic properties are determined by the distribution and relative movement of these nano-level spherical particles. The kinetic theory is an ideal tool to describe molecular level nanofluid problems. According to the kinetic theory, the Boltzmann equation provides a general description of a time-rate change of distribution function  $f$ ,

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{c}} = C(f) \quad (1)$$

where  $\mathbf{c}$  is the particle velocity,  $\mathbf{F}$  is the total force acting on the particle,  $m$  is the mass of the particle, and  $C(f)$  is the collision integral term. The singlet distribution at location  $\mathbf{r}$  with velocity  $\mathbf{c}$  at time  $t$  in the phase space is  $f = f(\mathbf{r}, \mathbf{c}, t)$ . The Chapman-Enskog perturbation method [1, 2] is adopted here to obtain analytical solutions for the viscosity and thermal conductivity of a nanofluid. If  $f_0$  stands for the distribution function at equilibrium, we replace  $\mathbf{c}$  by the peculiar velocity  $\mathbf{C} = \mathbf{c} - \mathbf{c}_0$ , where  $\mathbf{c}_0$  is the stream velocity,  $f$  can be expressed as

$$f = f_0(\mathbf{r}, \mathbf{C})[1 + \psi(\mathbf{r}, \mathbf{C})] \quad (2)$$

where  $\psi(\mathbf{r}, \mathbf{C})$  is a perturbation function. Equations (1) and (2) can be solved by the Chapman-Enskog method and the perturbation part  $\psi$  may be expanded in terms of Sonine polynomials. The leading term contributes mainly to the physical properties of a nanofluid and the perturbation function may be written as

$$\psi(\mathbf{r}, \mathbf{C}) = -A(\mathbf{r}, \mathbf{C})\left[\left(W^2 - \frac{5}{2}\right)C \nabla \ln T\right] + B(\mathbf{r}, \mathbf{C})\left[\overset{o}{\mathbf{W}} \mathbf{W} : \nabla \mathbf{c}_0 + \frac{\Gamma}{3} C^2 \mathbf{U}(\mathbf{U} : \nabla \mathbf{c}_0)\right] \quad (3)$$

where  $T$  is the absolute temperature,  $\mathbf{U}$  is the unit dyadic,  $\mathbf{W} = \left(\frac{m}{2k_B T}\right)^{1/2} \mathbf{C}$ ,  $\overset{\circ}{\mathbf{W}} = \mathbf{W} - \frac{1}{3} \mathbf{U}(\mathbf{U} : \mathbf{W})$ ,  $\overset{\circ}{\mathbf{W}} \mathbf{W} = \left(\frac{m}{2k_B T}\right) \left(\mathbf{C} \mathbf{C} - \frac{1}{3} C^2 \mathbf{U}\right)$ ,  $\overset{\circ}{\mathbf{W}} \overset{\circ}{\mathbf{W}} = \left(\frac{m}{2k_B T}\right) \left(\mathbf{C} \mathbf{C} - \frac{1}{3} C^2 \mathbf{U}\right)$ ,  $\Gamma = \frac{m}{k_B T} \left(1 - \frac{p^0}{k_B n T}\right)$ ,  $n(\mathbf{r})$  is the particle number per unit volume,  $m$  is the mass of the particle,  $k_B$  is the Boltzmann's constant,  $A(\mathbf{r}, \mathbf{C})$  and  $B(\mathbf{r}, \mathbf{C})$  are coefficients, determined by the pertaining kinetic equation, and  $r = |\mathbf{r}|$ . From the corresponding definition in the continuum fluid mechanics  $q = -K \nabla T$ , the thermal conductivity  $K$  can be obtained from (3) as

$$K = \frac{2k_B^2 T}{m} A_K(\mathbf{r}), \quad A_K(\mathbf{r}) = \int f_0 W^2 (W^2 - \frac{5}{2}) \mathbf{W} \mathbf{W} d\mathbf{c} \quad (4)$$

From the knowledge of fluid mechanics, the expressions for the corresponding stress components can be expressed in terms of viscosity  $\mu$  and second viscosity  $\eta$ . Thus, the pressure tensor is

$$\boldsymbol{\tau} = -p \mathbf{U} + 2\mu \overset{\circ}{\nabla} \mathbf{c}_0 + \lambda \mathbf{U}(\mathbf{U} : \nabla \mathbf{c}_0), \quad \overset{\circ}{\nabla} \mathbf{c}_0 = \nabla \mathbf{c}_0 - \frac{1}{3} \mathbf{U}(\mathbf{U} : \nabla \mathbf{c}_0) \quad (5)$$

The final expression for viscosity is obtained as  $\mu = \frac{nk_B T}{5} B_\mu(\mathbf{r})$  and the second viscosity  $\lambda = \frac{m\Gamma}{3} B_\lambda(\mathbf{r})$

where  $B_\mu(\mathbf{r}) = \frac{1}{n(\mathbf{r})} \int B(\mathbf{r}, \mathbf{C}) (\overset{\circ}{\mathbf{W}} \mathbf{W} : \overset{\circ}{\mathbf{W}} \mathbf{W}) f_0 d\mathbf{c}$ ,  $B_\lambda(\mathbf{r}) = \int f_0 B(\mathbf{r}, \mathbf{C}) C^2 \mathbf{C} \mathbf{C} d\mathbf{c}$ .

## NUMERICAL SIMULATIONS

We set the argon atoms on the upper wall at unit velocity along the x direction, and the atoms on the lower wall remain fixed, which induces a planar Couette flow in a nanopore. The simulation area is chosen as  $200 \times 100$  in the x and y directions. The temperature of fluid atoms is kept at 125K, which guarantees the argon in liquid state and a Nose-Hoover thermostat in the nanopore. The Verlet algorithm [3] is used to calculate the motions of molecules.

## CONCLUSIONS

Theoretical expressions for the thermal conductivity and the first and second viscosity coefficients are obtained. The results expressed in terms of the pair correlation function show some basic physical properties of nanofluids. The MD method with a complex model taking into account both the fluid-fluid and fluid-wall intermolecular interactions is further applied to simulate the Couette flow in a nanopore. The averaged viscosity values by the MD simulations are somewhat higher than those obtained from the kinetic theory. However, both are in qualitative agreement in the present study.

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## References

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