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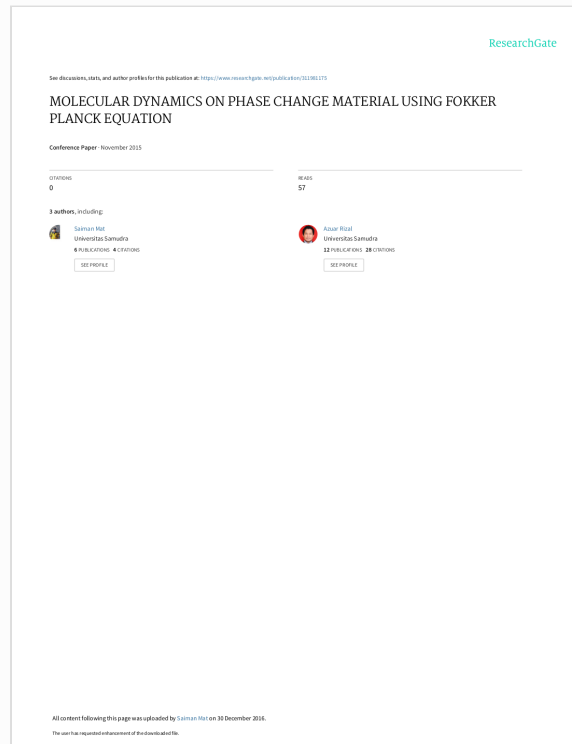
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MOLECULAR DYNAMICS ON PHASE CHANGE MATERIAL USING FOKKER PLANCK EQUATION

Conference Paper · November 2015

Molecular Dynamics on Phase Change Material Using Fokker Planck Equation

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Abstract

It has been calculated molecular dynamics equations nanofluid on Phase Change Material uses Fokker Planck equation. Particle dynamics in nanofluid usually use the equation of Brownian motion which does not describe the interactions between the particles. Fokker Planck equation are components of particle diffusion and overview of the interactions between the particles, so that got nanofluid molecular dynamics equations that can describe the physical properties of Phase Change Materials

Key words: molecular dynamics, Phase Change Materials, Fokker Plank Equation

Introduction

Phase change/transition materials (PCM), with many good thermophysical properties in thermal energy storage, have been widely investigated and applied in industrial areas for energy saving (Rao, Wang, Wu, Zhang, & Li, 2012). Energy in the form of heat can be stored in a state of sensible heat or latent heat or with a combination of both. The storage temperature depends on its use. Storage temperature can be classified as low (less than 100 ° C), medium (100 to 450 ° C) and high (higher than 450 ° C). Storage time can be classified as short duration (a few hours to several days) and long duration (a few months to a few seasons). Sensible heat storage is done by adding energy to the material to increase the temperature without changing the phase. The material used can be either liquid or solid. The most commonly used fluid is water and oil. The solid material is often used as stone, brick, concrete, iron, dry and wet soil, and many others.

According to Lane (1984), storage of latent heat energy requires a smaller volume than the sensible heat energy storage. Besides, the energy storage of latent heat can store a large amount of heat energy with small changes in temperature, however, the energy storage of latent heat still has a lot of problems about the materials used to make the process of energy storage such as high costs, low thermal conductivity and stability on thermophysics properties after processing cycles (recurrent). When the particles collide so that the particles slowed down or gets the frictional forces, hence condition Lioville equation can not be used. Instead the evolution of the distribution function is replaced by Fokker-Plank equation. Occurred as a result of collisions between the particles, the particles move randomly change. Particle called a Brownian particle has the distribution function $f(\bar{r}, \bar{v}, t)$ and experience the process of diffusion. Random particle motion and particle motion is not influenced by the movement of the particles beforehand.

Phase Change Materials

Sensible heat storage material must have high thermal properties, namely the specific heat Cp, density, thermal diffusivity α. Material storage should be repeated (reversible) as many cycles during hot filling (charging) and disposals/discharging. The amount of heat energy that can be stored on the state of the sensible heat can be calculated using the equation:

$$Q = \int_{T_1}^{T_2} m * C_p * dT = m * C_p * (T_2 - T_1)$$

Where "Q" is the amount of heat energy that can be stored on the state of the sensible heat (kJ), "T1" is the initial temperature (ₒC), "T2" is the final temperature (ₒC), "m" is the mass of the material that is used as a medium heat storage (kg), and "CP" is the specific heat of the material used as the heat storage medium (kJ/kg.ₒC). Based on this equation it is clear that the amount of heat energy that can be stored in a state of sensible heat depending on the mass, specific heat value of the material and temperature changes. It is known that water is one of the best materials that can be used to store water because the sensible heat energy available in large amounts, cheap, has a specific heat and a high density. Until now, commercial applications are still using water as thermal energy storage in liquid-based systems. Latent heat storage utilizing the latent heat contained in the material to store thermal energy. Latent heat is the amount of heat absorbed during the change in the material from one phase to another phase. There are two known types of latent heat is latent heat of fusion and the latent heat of vaporization.

Latent heat of fusion is the amount of heat absorbed when the material changes from a solid phase to a liquid phase or vice versa, then the latent heat of vaporization is the amount of heat energy absorbed when the material changes from liquid phase to vapor phase or vice versa. Indeed latent heat of vaporization is not considered to latent heat energy storage applications because of the large changes in volume is accompanied by a phase change. The amount of thermal energy storage in latent heat is determined by:

$$Q = m * LH$$

Where "Q" is the amount of heat energy stored by the latent heat (kJ), "m" is the mass of material that is used to store thermal energy (kg), and "LH" is the latent heat of fusion or vaporization (kJ / kg). Based on

the equation it is clear that the amount of heat energy that can be stored in a state of latent heat depends on the mass and the value of the latent heat of fusion or the evaporation. The material used as a store of heat energy in a state of latent heat so-called Phase Change Materials (PCM). According to Lane (1984), storage of latent heat energy requires a smaller volume than the sensible heat energy storage. Besides, the energy storage of latent heat can store a large amount of heat energy with small changes in temperature, however, the energy storage of latent heat still has a lot of problems about the materials used to make the process of energy storage such as high costs, low thermal conductivity and stability on thermophysics properties after processing cycles (recurrent). All materials are Phase Change Materials (PCM). The most important difference between this material is in the form of changes in temperature.

Each material change form (phase) at different temperatures. Besides, each material also has a different value of the latent heat and thermal conductivity. The major drawback of most of PCM is the low thermal conductivity will decrease the rate of heat transfer. The most important trait in selecting PCM is a phase change material that has a temperature which is accompanied by changes in the temperature range. Indeed, no specific material is referred to as an ideal material for use as PCM, the material has advantages and disadvantages of each.

Fokker Planck equation

Fokker-Planck equation is an equation that describes the distribution function of particles in a system that contains many particles collide (Palupi, 2010). This equation was first introduced by Fokker and Planck. Several application of the Fokker-Planck equation, among others on the erratic movement of small particles immersed in a fluid, fluctuations in the intensity of the laser beam, and the velocity distribution of fluid particles in turbulent flow. In general, the Fokker-Planck equation can be applied to the system of balance and imbalance (Frank, 2004). The initial formation of nonlinear Fokker-Planck equation is the result of collision between particles, thus changing the direction of motion at random (Brownian Motion). Particle called a Brownian particle is undergoing a process of diffusion. Random particle motion and particle motion is not affected by previous particle motion (Palupi, 2010). Fokker-Planck equation including partial differential equations (PDE) because these equations describe the rate of change of the two independent variables are time and distance (space). If seen from the equation (1), then the Fokker Planck equation is a PDE-order one of the independent variables t and a second order of the independent variables x. Fokker Planck equation is a parabolic-type PDE.

Fokker-Planck equation is an equation that describes the distribution function of particles in a system that contains many particles collide with each other. This equation contains diffusion component particles and interactions between particles (Palupi, 2010). The general form of the Fokker-Planck equation is with v the particle distribution function, A called floating coefficient (drift coefficient) and B called diffusion coefficient (Zauderer, 2006). Fokker-Planck equation including partial differential equation because it contains partial derivatives, ie derivatives with two independent variables x and t. One method to solve partial differential equation is the line method (method of lines). Line method is a specific finite difference method which produces a numerical solution to approach the actual solution. The basic idea of this method is to change the form of partial differential equations in the form of ordinary differential equations.

As a result of collision between the particles, the particles change direction at random motion. Particle called a Brownian particle distribution functions $f(\bar{r}, \bar{v}, t)$ and has undergone a process of diffusion. Random particle motion and particle motion is not influenced by particle motion said that before or in other words, the particles can no longer remember the previous movement (Medhi, 1982; Schuss, 1980). In other words, the particles follow a Markov process. If the shift of the particle at a time is $X(t)$ and the probability distribution function is expressed in transition from the current position x_0 at s to x at the time t is s <t., Then the transition probability density or distribution function is given by

$$p(x_o, s, x, t)\, dx = Pr\{x \le X(t) < x + dx | X(t_0) = x\}$$

with

$$P(x_o, s, x, t)\, dx = Pr\{x \le X(t) < x + dx | X(t_0) = x\}$$

For a homogeneous process of transition probability density depends only on the lapse interval *(t - s)*, the transition probability density can be expressed x_0, x, *(t-s)* only. So that only the parameters $Pr\{x \le X(t) < x + dx | X(t_0) = x\}$ can be expressed as $p(x_o, s, x, t)\, dx$ to any t_0. Based on Chapman-Kolmogorov equation then meetings transition probabilities can written as follows :

$$p(x_o, s, x, t)\, dx = \int p(x_0, s; z, v) p(z, v, x, t)\, dz$$

Suppose Brownian particles in a short time interval · x · t shifted so far, the total shift in time *t* is $X(t)$ after *N* steps is expressed as

$$X(t) = \sum_{i=1}^{n} Z_i$$

Z_i is a random variable that specifies the length or distance in step *i*. The time required for each step is · t, then the number of steps is $N = (t/\Delta t)$. Distance occur at each stage can be +· x which means that the particles move forward or be · x which means particles moving backwards. Probability distance +· x can be exemplified as the probability *p* and distance -· x can be exemplified as *q*. Total probability of both movements thus = *p + q* = 1.

Fokker Planck equation that describes the evolution of distribution because of weak collisions causing minor shifts can be served in the room rate. If *f* is the distribution function does not depend on space $f(v, t)$ · than Fokker-Planck equation in the form (Kirk, 2002;Somov, 2003)

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}(a(x,t)p) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(b(x,t)p)$$

$$\left(\frac{\partial f}{\partial t}\right)_c = -\frac{\partial}{\partial v}[a_\alpha f] + \frac{\partial^2}{\partial v_\alpha \partial v_\beta}[b_{\alpha\beta} f]$$

Coefficient a is the coefficient of dynamic friction. Brownian particle gets frictional forces against the movement and the coefficient b is a diffusion coefficient that is the average change of pace. The first tribe -Planck Fokker equation is a friction that slows the beam of particles and the particles move towards zero

velocity in the phase space, while the second form of diffusion presents a beam of particles in three-dimensional space velocity.

Application Fokker Plank Equation In Molecular Dynamics PCM

Space in the PCM is composed of a fluid system. Fluid system composed of ions, which can be charged positively or negatively or positively charged and negatively so that the total charge is 0 or a neutral fluid. Because the fluid system composed of ions, the Coulomb interaction between the particles making up the fluid. Collisions in a fluid can not be determined uniquely as the neutral atoms (Bennz, 2002). Coulomb potential interactions with other particles gives the effect that the first two test particles moving in a fluid experience deviations from the original direction, which both accelerate particles terrain. The influence of the latter accounted for a loss of energy and provide frictional forces on the motion of test particles. Both of these effects depends on the ratio of the two particles. Review the fast particle beam in a fully ionized fluid thermally gets the internal magnetic field H_0. An internal magnetic field that determines the course of the particle. Suppose tesusun fluid on thermal electrons and protons that are in thermodynamic equilibrium and v is the particle distribution function test of the equations of motion of a particle is (Somov, 2003).

$$\frac{df}{dt} + v_\alpha \frac{\partial f}{\partial r_\alpha} + \frac{q}{m}\{v \times H_0\}\frac{\partial f}{\partial v_\alpha} = -\frac{\partial f}{\partial v_\alpha}J_\alpha$$

When viewed in a stationary state, and only depends on the variables of space alone or with a z-shaped field direction **H₀**, $f = f(z, v, \theta)$ form

$$v \cos\theta \frac{\partial f}{\partial z} = \frac{1}{v^2}\frac{\partial}{\partial v}(v^2 J_v) - \frac{1}{v\sin\theta}\frac{\partial(\sin\theta J_\theta)}{\partial\theta}$$

by equating with the Fokker-Planck equation becomes

$$x \cos\theta \frac{\partial f}{\partial\delta} = \frac{\partial F(x)f}{\partial x} + \frac{\partial^2}{\partial x^2}[D(x)f] + D_\theta(x)\Delta_\theta f$$

The first coefficient on the *F(x)* which determines the energy loss when the accelerated particles through the fluid. The second coefficient is *D(x)* describe the diffusion of energy. The third *D₀(x)* coefficient associated with particle diffusion quickly on Considering the electron mass is much smaller than the mass of the electron. In this case, the coefficient on Fokker Plank equation becomes:

$$D(x) = \frac{1}{\sqrt{x}}\left(1 + \frac{m_e}{m_p}\right)$$

$$F(x) = -\frac{m}{m_e}\frac{1}{\sqrt{x}}\left(1 + \frac{m_e}{m_p}\frac{1}{x}\right)$$

$$D_\theta(x) = \frac{1}{2x\sqrt{x}}$$

The first tribe in the coefficient D (x) Brazilians donated fluid thermal collisions between electrons, while the second term is the contribution to the thermal protons. The first two show the energy coefficient of

diffusion due to collisions with electrons m_p/m_e thermal more than proton because of collisions with thermal. While the speed of diffusion angle is determined equally by the electron and proton fluid. Test particle velocity distribution in the fluid can be determined by using the Fokker Planck equation in space speed. Review the set of test particles with the same speed that is easy to move, test particle velocity distribution d approached isotropic before loosing power. If the particles are mobile field, drag on the particle slows the particles before the turn. The time between the test particles begin to change the direction of movement is generally different from the time when the particles lose power or lose momentum.

Conclusions

Fokker Planck equation is a diffusion equation that describes the distribution function of particles in a system that contains many particles collide with each other. The equation can be used in molecular dynamics recall PCM in the form of a fluid chamber, which is composed of charged particles. Particle motion and diffusion processes in the plasma can be solved by using the Fokker Plank equation in the coordinate space and in space velocity. Scattering, interaction and diffusion process occurs not only because of the interaction between the particles but also the interaction between the particles and electromagnetic.

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