Dynamics of nanoparticle concentration in nanofluids under laser light field

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Abstract. The dynamics of the concentration of nanofluids placed in a light field with a Gaussian intensity profile is studied theoretically. The investigation is based on the analytical and numerical solutions of the system of linearized heat conduction and convection-diffusion equations. The convection-diffusion equation contains terms that correspond both to the Soret effect and to the transfer of nanoparticles, caused by the action of a light field on them (electrostriction). The dependence of the coefficient of thermal conductivity of the medium on the concentration is taken into account. It is shown that under these conditions single travelling waves appear in the medium, the velocity of which depends not only on the thermal physical parameters of the medium, but also on the polarization of the particles. Conditions under which the stratification of the medium is possible are found.

1. Introduction

Colloidal suspensions or, as they are now called, nanofluids, are widely used in various areas of modern technology. For example, magnetic fluids are used to polish optical components, and suspensions of silica particles in liquid crystals significantly improve the characteristics of optical storage devices [1-2]. We also note their use in chemical processes (catalysis), in the creation of new drugs, lubricants and so on [3-7]. With the growth of the productivity of electronic devices and the development of high-energy technologies, it has become necessary to create efficient cooling systems and control large heat flows [8]. Promising developments have emerged related to molecular computers based on switchable bistable molecules or their aggregates. One way to intensify heat transfer is to increase the thermal conductivity of a liquid by adding solid particles with high thermal conductivity [9-12].

Particularly interesting for the creation of such suspensions are nanoparticles. Recent studies have shown that liquid-phase media, in which nanoparticles from wide-gap semiconductors or dielectrics are used as a dispersive component, are very effective for the realization of a number of nonlinear optical effects [13]. In these media, unlike homogeneous media, the nonlinear optical response arises from the change in the refractive index induced by the light wave and the absorption coefficient due to the phenomena of thermal diffusion and electrostriction of particles [14-18]. At the same time, in our opinion, physical mechanisms connected in particular with the processes of heat and mass transfer in such media require additional investigation. It should be added that a number of mathematical
problems associated with analytical methods for solving the corresponding equations are also far from being resolved.

2. Theoretical model

The paper considers a liquid-phase medium with nanoparticles irradiated by a light beam with a Gaussian intensity profile. As a result of the action of the light field in the medium, gradients of temperature and concentration arise, which cause the processes of heat and mass transfer. These phenomena are described by a system of balance equations for temperature and particles, taking into account the concentration convection [19], written in one-dimensional form (without using the Boussinesq approximation):

\[
C_p \rho \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \lambda(C) \nabla T \right) + a_0 I_0 \exp\left(-\frac{x^2}{\sigma^2}\right),
\]

(1)

\[
\frac{\partial C}{\partial t} = D \nabla^2 C - \nu \nabla C + D_C \nabla (C(1-C)\nabla T) - \gamma \frac{\partial}{\partial x} \left( C \frac{\partial T}{\partial x} \right),
\]

(2)

In the heat equation, the term responsible for the Dufour effect is omitted, in view of its smallness. The processes of sedimentation are also neglected. Here, the following designations are used: \( T \) is the temperature of the medium, \( C = C(r,t) = m_0/m \) is the mass concentration of the particles (\( m_0 \) is the mass of the particles, \( m \) is the mass of the whole medium), \( C_p, \rho \) are the thermophysical constants of the fluid, \( \lambda(C) \) is the coefficient of thermal conductivity, \( I_0 \) is the light intensity, the absorption coefficient of the medium, and the diffusion and thermal diffusion coefficients, respectively, and \( \nu = \eta/h \) is the rate of concentration convection, which we assume to be constant. In this case, \( \eta \) is the kinematic viscosity, and \( h \) is the characteristic distance (in our case, we take \( h \approx 10x_0, \gamma = 4\pi\beta D/(c n_{ef} k_B T) \), \( \beta \) is the polarizability of the particles, \( k_B \) is Boltzmann’s constant, \( c \) is the speed of light in vacuum, \( n_{ef} \) is the effective refractive index of the medium. The last term expresses the contribution from the particle flux and is related to the effect of the gradient force from the side of the light field (electrostriction of particles).

![Figure 1. Geometry of the problem (1 = cuvette; 2 = liquid medium with nanoparticle).](image)

Let us take into account the fact that the temperature establishment processes go faster than the diffusion processes. This makes it possible to study the latter against a background of a stationary temperature. We will consider the case of small concentrations: \( C \ll 1 \).

Further, the concentration dependence of the thermal conductivity can be represented in the form:

\[
\lambda(C) = \lambda_o + \beta C = \lambda_o (1 + pC),
\]

where \( p = \frac{\beta}{\lambda_o} > 1 \). This kind of dependence was theoretically found in [20] and was experimentally confirmed in publications [21, 22]. In the equations of heat conduction and diffusion, divergent terms are taken in the form:

\[
\]
\[
\frac{\partial}{\partial x} \left( \lambda(C) \frac{\partial T}{\partial x} \right) \approx \lambda(C) \frac{\partial^2 T}{\partial x^2}, \quad \gamma \frac{\partial}{\partial x} \left( C \frac{\partial I}{\partial x} \right) \approx \gamma C \frac{\partial^2 I}{\partial x^2}.
\]  
(4)

The validity of this approximation for the first formula is based on the use of equality (3), which leads to a reasonable inequality, \( pC < 1 \), and for the second, it is justified by direct estimates of the quantities. Next, we linearize equation (2), step by step. First, we assume:

\[
(\lambda(C))^{-1} = (\lambda_0 + \beta C)^{-1} = (\lambda_0)^{-1} (1 - pC). \quad (pC \ll 1)
\]  
(5)

Assuming that \( C \ll 1 \), we represent the concentration in the form:

\[
C(x,t) = C_0 + \Delta C(x,t) = C_0 (1 + C'(x,t)) \quad C'(x,t) = \frac{\Delta C}{C_0},
\]  
(6)

where \( \Delta C(x,t) \) is the disturbed part of the concentration, and \( |\Delta C| \ll |C_0| \) approximations (3), (4) and its linearization with respect to the function \( u(x,t) = 1 + C'(x,t) \), we obtain the problem. After substituting expressions (5) and (6) into equation (2), taking into account the:

\[
\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} - \frac{D_T \alpha_0}{\lambda_0} (1 - pC_0) \exp(-\frac{x^2}{x_0^2})u + \frac{4\gamma T_0}{x_0^2} (1 - \frac{x^2}{x_0^2}) \exp(-\frac{x^2}{x_0^2})u
\]  
(7)

\[
u(x,0) = \exp(-\frac{x^2}{x_0^2}), \quad \frac{\partial u(0,t)}{\partial t} = 0, \quad 0 \leq x < \infty.
\]  
(8)

We rewrite the problem (7)–(8) in dimensionless variables:

\[
\frac{\partial u}{\partial \tau} = \frac{b}{\rho^2} \frac{\partial^2 u}{\partial \rho^2} - Peb \frac{\partial u}{\partial \rho} + (q(1 - \rho^2) - 1) \exp\left(-\rho^2\right)u,
\]  
(9)

\[
u(\rho,0) = \exp(-\rho^2), \quad \frac{\partial u(0,\tau)}{\partial \rho} = 0, \quad 0 \leq \rho < \infty, \quad 0 \leq \tau < \infty,
\]  
(10)

where \( \tau = \frac{S \alpha_0 \lambda_0 D}{\lambda_0} (1 - pC_0) t, \quad \rho = \frac{x}{x_0} \), \( Pe = \frac{v x_0}{D} \), \( Peclet number, \quad b = \frac{\lambda_0}{S \alpha_0 \lambda_0 (1 - pC_0) x_0 \tau} \), \( q = \frac{4\gamma T_0}{D} b \).

It is not possible to find the exact analytic solution of equation (7) with initial-boundary conditions (8). The Peclet number estimate for typical values of the quantities in our case gives \( Pe \geq 10^3 \).

This value indicates the predominance of convection processes over molecular diffusion. In view of this fact, we rewrite problem (7)–(8) in a truncated form:

\[
\frac{\partial u}{\partial \tau} = -Peb \frac{\partial u}{\partial \rho} + (q(1 - \rho^2) - 1) \exp\left(-\rho^2\right)u,
\]  
(11)

Its exact solution can be written in the form:

\[
u(\rho, \tau) = A \exp[-(\rho - Peb \tau)^2] \exp\left[-\frac{1}{4Peb} \sqrt{\pi (q - 2) \text{erf}(\rho) + 2q \rho \exp(-\rho^2)}\right],
\]  
(12)

where \( \text{erf}(\rho) \) is the error function (Gauss). The constant \( A \) can be determined from the condition of conservation of the number of particles in the system.
Figure 2 shows the graphs of the function $u(\rho)$ at increasing times $\tau$.

![Graph of $u(\rho)$](https://example.com/graph.png)

Figure 2. The graphs of the solution $u(\rho, \tau)$ presented for different instants of time (as they increase).

Thus, accounting for the concentration convective flow, even in the one-dimensional approximation, leads to amplitude-modulated travelling waves.

Let us now consider the state of mechanical equilibrium of a nanofluid, that is, when its macroscopic flow is absent and the equilibrium distributions of temperature and concentration are described by the equations:

\[
\nabla^2 T + \frac{\alpha_{\rho}I_{0}}{\lambda_0} \exp\left(-\frac{x^2}{x_0^2}\right) = 0, \quad T(0) = T_0, \tag{13}
\]

\[
\frac{dC}{dx} + (S + \frac{\gamma}{D}) \frac{dT}{dx} = 0. \tag{14}
\]

The solution of this system is the expression:

\[
C(x) = B \exp[-S_iT_0 + n\rho\text{erf}(\rho) + (n + m)\exp(-\rho^2)], \tag{15}
\]

where $n = \frac{\alpha_{\rho}I_{0}S_i}{2\lambda_0}$, $m = \frac{2\bar{T}_{0}\gamma}{D}$.

The constant $B$ in formula (15) can be determined from the condition of constancy of the average concentration.

3. Discussion

Note that the convective processes in a colloidal suspension of nanoparticles taking into account sedimentation (in the Benard scheme) were studied in [23-25]. The mode of running concentration waves was detected. In our approach, the effect of radiation due to the action of gradient forces on the side of the light field, being an additional source of convection, leads to a completely different spatial distribution of concentration. We note that the amplitudes of the modulated waves in solution (12) are damped and have a spatially complex structure. In particular, an analysis of the exponent shows that with positive thermal diffusion ($b > 0$) and a change in the sign of the polarization of the particles $\beta$, its structure significantly changes (figure 3). These observations indicate the possibility of controlling the optical properties of nanofluids, since the nonlinear part of the refractive index of such a medium depends on the concentration.
Solution (15) shows that in our case the convection of a nanofluid has two processes: thermal diffusion and electrostriction, which can be either unidirectional or multidirectional. It is easy to see from (15) that if the contribution from electrostriction is small (m \ll n), then in the conditions of mechanical equilibrium, the resulting stratification (stratification) is associated with thermal diffusion.

We understand that a number of questions require more detailed study, for example, analysis of convection stability, numerical modelling of these processes and their study in a 2D measurement. We will devote our attention to these problems in future research.

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