The formation process of a bistable state in nanofluids

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Abstract. We study the theory of the dynamics of the concentration of nanoparticles in a liquid-phase environment under the influence of a light field. An exact solution for the nonlinear diffusion equation was found in the form of switching waves. It is shown that under the conditions of a stationary and nonlinear temperature coefficient of thermal conductivity of the medium, nanofluids become bistable.

1. Introduction
Nanoscale objects are a very popular subject for researchers because these systems have very specific properties [1–5]. Colloidal suspensions, or nanofluids as they are called today, are widely used in various fields of modern technology. For example, the magnetic fluid is used to polish optical components [6] because a slurry of silica particles in the liquid crystal substantially improves the characteristics of the optical drive [7]. Let us also note their use in chemical processes (catalysis) and the creation of new drugs, lubricants and so forth. With the increasing performance of electronic devices and the development of high technologies, it is necessary to create effective cooling systems and to manage large heat flows. One very promising development is related to molecular computers, which are based on switchable bistable molecules or their aggregates [8].

One of the ways to intensify heat transfer is to increase fluid thermal conductivity by adding solid particles with high thermal conductivity. Of particular interest in the creation of such suspensions are nanoparticles [9–12]. As shown by recent studies [8–15], the liquid phase of the medium, in which the components such as the dispersed nanoparticles are taken from wide bandgap semiconductors and dielectrics, are very effective for a number of nonlinear optical effects. In these media, unlike in homogeneous ones, the nonlinear optical response occurs due to light-wave induced changes in the refractive index and absorption coefficient, thermal diffusion phenomena due to electrostriction of particles. At the same time, the physical mechanisms involved, in particular the heat and mass transfer processes in these media, require further study in our view.

2. Theoretical model
The aim of our work is to conduct a theoretical study of the dynamics of nanoparticle concentration in the liquid-phase medium to be subjected to laser radiation of constant intensity, taking into account the thermal conductivity of the medium depending on its concentration. We believe that the size of the particles satisfies the condition: $a_0 << \lambda$, where $a_0$ is its linear size and $\lambda$ is the wavelength of the light. Thus, we do not consider diffraction and scattering processes. We also assume that the density of the liquid and the particles are nearly the same, giving the option to exclude sedimentation processes from consideration.

We consider the liquid-phase medium with microparticles irradiated with a light beam evenly distributed over the cell intensity. As a result of the light field in the medium, temperature and
concentration gradients occur, causing heat and mass transfer processes. These phenomena are described by the system of balance equations for temperature and particles [16]:

\[ C_p \rho \frac{\partial T}{\partial t} = \lambda \nabla^2 T + \alpha I_0, \quad (1) \]

\[ \frac{\partial C}{\partial t} = D \nabla^2 C + D_T \nabla \left[ C (1 - C) \nabla T \right]. \quad (2) \]

Note that in the heat equation (1), we have omitted the term responsible for the Dufour effect, because of its smallness, and in the diffusion equation (2) we do not consider a term corresponding to the action of gradient forces from the light field at this stage of research. The following notations are adopted:

- \( \nabla \) is the Laplace operator,
- \( T \) is the ambient temperature,
- \( C = C(r, t) = \frac{m_0}{m} \) is the mass concentration of particulate matter (\( m_0 \) is the mass of the particles, \( m \) is the mass of the entire environment),
- \( C_p, \rho \) and \( \lambda \) are the permanent thermal fluid properties,
- \( I_0 \) - the intensity of light,
- \( \alpha \) - optical absorption coefficient of the medium and \( \lambda_D, T_D \) are the diffusion coefficients and thermal conductivity, respectively.

In such a general statement of the system, (1) and (2) are unlikely to be solved. Therefore, we make some simplifying assumptions: we consider the one-dimensional case and exclude the contribution of the convective term, which occurs in equation (2). Then we take into account the fact that the processes of establishing the temperature goes much faster diffusion process. This makes it possible to study the diffusion processes at a fixed temperature: \( \frac{\partial T}{\partial t} = 0 \). In equation (1), we assume that the thermal conductivity depends on the concentration and that this dependence has the form [10, 11]:

\[ \lambda(C) = \lambda_0 + \beta C = \lambda_0 (1 + p C), \quad (3) \]

where \( p = \frac{\lambda'}{\beta} \) is the coefficient of proportionality. Note that this type of dependence was observed in a number of experiments [14]. Given the above, the diffusion equation (2) can be written as:

\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - D_T \frac{\alpha I_0}{\lambda(C)} C (1 - C). \quad (4) \]

Proceeding in this equation to the dimensionless variables, we obtain:

\[ \tau = \frac{S_T}{\lambda_0} I_0 \alpha D t, \quad y = x \sqrt{\frac{S_T}{\lambda_0} I_0 \alpha}, \quad S_T = \frac{D_T}{D} \] - Soret coefficient. If we also use the approach \( \frac{1}{\lambda(C)} \approx \lambda_0 (1 - p C) \), we obtain the problem:

\[ \frac{\partial C}{\partial \tau} = \frac{\partial^2 C}{\partial y^2} - p C^3 + (1 + p) C^2 - C, \quad (5) \]

\[ 0 \leq C \leq 1, \quad -\infty < y < \infty, \quad 0 \leq \tau < \infty. \quad (6) \]
Such parabolic equations with cubic nonlinearity were considered in [16, 17] for modelling dissipative media. First, we consider spatially homogeneous stationary states. Obviously, the zeros of the source function in equation (5): \( C_1 = 0, C_2 = 1/p \) \( (p > 1), C_3 = 1 \) correspond exactly to such states.

It is known that the kinetics of the dissipative system are highly dependent on the stability of the stationary states. In our case, the state \( C = C_3 \) is stable (they are derived from the source \( F'(C) < 0 \) and the state \( C = C_2 \) is unstable. Thus, we found that the medium is bistable. Following [17], the solution of equation (3) will be found by substituting the Cole-Hopf:

\[
C(y, \tau) = \frac{u(y, \tau) \mu}{u(y, \tau) + u_0},
\]

where \( u(y, \tau) \) is a new function and \( \mu, u_0 \) are constant.

Substituting (7) into (5) and equating to zero the coefficients of the same powers of a system of linear equations to determine \( u(y, \tau) \), we obtain:

\[
\begin{align*}
\mu &= \pm \sqrt{2} p. \\
\end{align*}
\]

The characteristic equation corresponding to (9) can be written as:

\[
k \left[ 2k^2 - (\text{sgn } \mu) \cdot (1 + p) k + 1 \right] = 0,
\]

its roots: \( k_0 = 0, k_1 = \frac{1}{\sqrt{2} p}, k_2 = \frac{p}{\sqrt{2}}. \)

Further, given the symmetry of the equation (5) with respect to the replacement \( y \rightarrow -y \), we restrict ourselves to a positive value of \( \mu \). Therefore, for the function we have:

\[
\mu(y, \tau) = a_0 + a_1(\tau) \exp(k_1 y) + a_2(\tau) \exp(k_2 y)
\]

Substituting (11) into (9) we find:

\[
a_0 = A_0, \ a_i(\tau) = A_i \exp(\eta_i \tau), \ \eta_i = 3k_i^2 - k_i(1 + p) \sqrt{\frac{p}{2}} , i = 1,2.
\]

where \( A_i \) are the constants determined from the initial conditions.

Thus, the exact solution of the equation (5) will have the form:

\[
C(y, \tau) = \sqrt{2} p \frac{N_1 k_1 \exp(k_1 y + \eta_1 \tau) + N_2 k_2 \exp(k_2 y + \eta_2 \tau)}{1 + N_1 \exp(k_1 y + \eta_1 \tau) + N_2 \exp(k_2 y + \eta_2 \tau)},
\]

where

\[
N_i = \frac{A_i}{(a_0 + z_0)}.
\]

Note that such a solution was obtained by another method in [18].
3. Results and conclusions

Obviously, the solution (13) is continuous for any values and we note that solution (13) describes a bistable dynamics system, in which a wave state of the switching system is formed by a two-beam mechanism. Thus, phase ‘partial’ waves are linearly independent.

Passing from the exponent in (13) to the dimensional variables, we obtain the expression for the wave velocities:

\[
\nu_{1,2} = \sqrt{\frac{S_1 I_0 \alpha}{\lambda_0}} \left(1 + \frac{p}{2} - 3k_{1,2} \right) D \tag{14}
\]

Given that \( p > 1 \), and the expression for \( k_{1,2} \), it is evident that this ‘two-phase’ solution is a concentration of two plane waves with speeds of \( \nu_{1,2} \). Thus, the exact solution of (14) describes the interaction of two concentration waves switching from the intermediate unstable state \( (C_2 = 1/\rho) \) to the stable state \( (C_1 = 0, C_3 = 1) \). Further, since \( \eta_1 > \eta_2 \), then we finally have:

\[
C(y, \tau) \approx \sqrt{2p} \frac{N_k \exp(k_1 y + \eta_1 \tau)}{1 + N_k \exp(k_1 y + \eta_1 \tau)}.
\]

Note that if we consider the diffusion processes against a background of a fixed temperature with a constant coefficient of thermal conductivity, equation (3) is transformed into a well-known Kolmogorov-Petrovskii-Piskunov (KPP) equation [19], which, as we know, has only a single-wave solution. It is important, in this case, that the system loses its bistability (there are only two spatially homogeneous stationary states).

Of course, our approach is to some extent a model; nevertheless, the authors hope they have managed to discover under which conditions irradiated nanofluids acquire the properties of a dissipative bistable medium in which can propagate a switching wave.

We believe that not all of the issues have been exhaustively studied; for example, an inverse relationship between temperature and the concentration of nanoparticles in the dynamics of the system, taking into account the absorption coefficient of the concentration, was not considered. A detailed examination of this topic will be the subject of our further research.

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