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Nonlinear wave model for transport phenomena in media with non-local effects

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The purpose of the work is to establish and substantiate the prerequisites under which the modified Whitham equation can play the role of a transfer equation in physical-chemical systems and technological processes.
The contribution of this work lie in the fact that the perturbed Whitham equation describing propagation of nonlinear waves in media with non-locality has been derived using the nonlinear relaxation function. It is shown that while deriving the equations of the Whitham type, the presence of the spatial non-locality of the medium can play a fundamental role. The paper also considers the issues of physical interpretation of the model under study. The principal presence of non-local effects in studied systems can be substantiated and obtained as a result of the presence of domains with a complexly organized spatial structure as well as in the presence of heat and mass sources. The new model submitted in the work can find application in methods for calculating the intensity of heat and mass transfer in complexly structured heterogeneous systems.

1. Introduction

Accounting of the relaxation times and long-range interactions of structural elements of media while mathematical modelling the mass, heat and momentum transfer are of great scientific and practical interest (Sobolev, 1994, Karličić et al., 2015). Similar problems also arise when describing the development of internal stresses and the formation of cracks in solids (Martowicz et al., 2014, Diehl & Schweitzer, 2015). These issues are especially relevant for mathematical modelling the high-intensity technological processes when correctness of the methods of equilibrium thermodynamics becomes problematic (Mansard et al., 2013, Lyakhovsky et al., 2011). At the same time, the methods of non-equilibrium thermodynamics, when applied in full form (Jou et al., 2001), are too complex both for calculating the control parameters, and for analysis of the qualitative state of the system. For fast processes the selection of the transient stage and the stage of stable control parameters becomes uncertain (Cheng-Chuan Lin & Fu-Ling Yanga, 2020). When modeling transport processes in nanosystems, the account of the nonlocality of the transport laws becomes unavoidable (Sundararaghavan & Waas, 2011, Srinivasan Gopalakrishnan & Saggam Narendar, 2013). This concludes from the presence of domains with a complex spatial structure (Gao & Oterkus, 2019), especially with allowance for arising and transforming the clusters in different moments and different space locations (Lyakhovsky & Ben-Zion, 2014), and from the presence of heat and mass sources too (Kim & Brener, 1996).
The Whitham integral-differential equation (Whitham, 1999) is the model efficiently describing nonlinear waves in strongly dispersive media. The equation contains a characteristic nonlinearity of the convective type in combination with dispersion of an arbitrary type. However G.B. Whitham proposed his equation without derivation and specific interpretation. It was found (Brener, 2006) that an equation of this type can be derived when modelling heat and mass transfer with propagation of nonlinear waves in media with spatial non-locality on the base of the method of relaxation transfer kernels. Under the derivation the linear relaxation function has been supposed. However, this assumption is not consistent with the general nonlinearity of the developed models. Such an assumption can find some justification only in the case of the presence of a single spatially bounded source of perturbation of properties in a generally isotropic medium (Quing Du et al., 2018).
The main novelty and contribution of this work lie in the fact that the perturbed Whitham equation describing propagation of nonlinear waves in media with non-locality has been derived using the nonlinear relaxation

function. This fact significantly expands the possibilities of using the obtained equation in methods for calculating the intensity of heat and mass transfer in various heterogeneous systems.

2. Theoretical details

Let us introduce the local deviation u of the control parameter ν from the equilibrium state of the system. Such a parameter for thermal processes is temperature; for mass transfer processes, it is chemical potential; for the propagation of internal defects in solids, it is equilibrium internal stress (Picu, 2002) :

$$\Delta \nu = u \ . \tag{1}$$

Then the expression for the flow J of a substance at small deviations from equilibrium, taking into account nonlocal effects (Kim & Brener, 1998) can be written as follows (Brener, 2006):

$$J = \int_{\Omega} N(\theta, u) \nabla u(s,t) ds \ . \tag{2}$$

Here N is the kernel of the integral operator, $\theta = x - s$
Integrating by parts leads to the expression

$$J = \int_{\Omega} N(\theta, u) \nabla u(s,t) ds = uN(\theta, u)\big|_{\Gamma} + \int_{\Omega} u \frac{\partial N(\theta, u)}{\partial \theta} ds \ , \tag{3}$$

where Ω , Γ are the integration region and its bound.
Further transformations and derivation of equations are carried out in the approximation of weak non-locality in order to remain within the framework of equilibrium thermodynamics (Jou et al., 2001, Brener, 2006).
This restriction can be written as follows

$$\lim_{|\theta| \to \infty} N(\theta, u) = 0 \ . \tag{4}$$

Let us denote the derivative of the kernel in integral operator of Eq(3) as

$$G(\theta, u) = \frac{\partial N(\theta, u)}{\partial \theta} \ . \tag{5}$$

Expansion of operator (5) in a Taylor series in the vicinity of the equilibrium values of the control parameter reads

$$G(\theta, u) = \sum_{k} G_{(k)}(\theta) u^k \ . \tag{6}$$

The general form of the conservation law reads

$$\frac{\partial u}{\partial t} + \nabla J = I \ , \tag{7}$$

where I is the intensity of the substance source in the system.

Use of conservation law (7) with account of Eq(3) leads to the following equation

$$u_t = \nabla u_t \int_{\Omega} \left(\sum_{k} G_{(k)} u^{k+1} \right) ds = I \ . \tag{8}$$

For correctness of further transformations, it is necessary to set the commutation condition for the differentiation and convolution operators in Eq(8). Since at this stage of transformations the form of kernels in the integral operator is unknown, this condition will need to be further checked for a specific type of physically meaningful kernels. Then, Eq(8) can be rewritten in the form

$$u_t + \int_{\Omega} \left(\sum_k (k+1) G_{(k)} u^k \right) u_s ds = I \ . \tag{9}$$

Further development of the theory requires specifying the form of the kernels of the operator in Eq(9). To solve this problem, the first-order relaxation equation that is characteristic for relaxation problems in theoretical physics can be used (Brener, 2006). However, in order not to violate the logic of the nonlinear approach, here, in contrast to Brener's work, the relaxation equation is written in a general form.

$$\frac{d}{d\theta} G_{(k)}(\theta) + B_{(k)} \Phi\left(G_{(k)}(\theta)\right) = 0 \ . \tag{10}$$

Here $\Phi(\bullet)$ should be a positive non-decreasing function (Brener et al., 2009).
Using the expansion of $\Phi(\bullet)$ in power series Eq(10) takes the form

$$\frac{d}{d\theta} G_{(k)}(\theta) + B_{(k)} \sum_{i=1}^{\infty} \lambda_i G_{(k)}^i(\theta) = 0 \ . \tag{11}$$

Restriction by the first two terms of the series leads to the following equation

$$\frac{d}{d\theta} G_{(k)}(\theta) + B_{(k)} \left(\lambda_1 G_{(k)}(\theta) + \lambda_2 G_{(k)}^2(\theta) \right) = 0 \ . \tag{12}$$

Then, it can be shown that the physically meaningful form of the equation looks as follows

$$\frac{d}{d\theta} G_{(k)}(\theta) + Y_{1,(k)} G_{(k)}(\theta) \pm Y_{2,(k)} G_{(k)}^2(\theta) = 0 \ , \tag{13}$$

where $Y_{1,(k)} \geq 0$, and $Y_{2,(k)} \geq 0$.
Below three main cases are considered.
Let us consider case 1, when $Y_{2,(k)} = 0$.
The physical interpretation of this case can be given in the framework of a pseudo-isotropic medium, when the influence of domains with a complex structure quickly dies out and weakly manifests itself on large scales. This behavior is typical for media with a low concentration of the inclusive phase. Nevertheless, such an influence can theoretically manifest itself in the form of single wave fronts (Brener, 2006).
The simplest heuristic form of the coefficient $Y_{1,(k)}$ in this linear approximation reads (Brener, 2006)

$$Y_{1,(k)} = \varphi_{(k)} / r_{(k)} \ . \tag{14}$$

Here $r_{(k)}$ is the characteristic spatial scale for k - th order, and $\varphi_{(k)}$ is the some coefficient for k - th order. In order to be consistent with the weakly nonlinear approximation and accepted form of the flow equation (Eq(3)), the sequence of characteristic spatial scales should form a decreasing series. These scales can also evaluate characteristic sizes of domains with a complexly organized spatial structure (Iovane and Passarella, 2004, Pereira, 2018) and, for example, describe arising and transforming the clusters in different moments and different space locations with allowance for the cross effects (Kim, Brener, 1998). Since the kernels of the integral operator in the transport equation are obtained under the assumption of weak non-locality, the system has a natural small parameter $\varepsilon = r_{(0)} / R$. Here $r_{(0)}$ is the maximum radius that should be taken into account when describing non-local interaction (Naumkin & Shishmarev, 1994), R is the characteristic scale of the macroscopic system. The estimation for $r_{(0)}$ can be given on the base of considering the scale of inclusions that violate the isotropy of the medium properties. Such complex structure can be manifested in the form of particles of another phase or so-called perforation of the continuous medium (Pereira, 2018).
The solution of Eq(13) in case 1 with coefficient $Y_{1,(k)}$ in form (14) reads

$$G_{(k)}(\theta) = G_{(k)}^0(\theta) \exp\left(-\frac{\varphi_{(k)}}{r_{(k)}} |\theta| \right) . \tag{15}$$

It can be easily proved that condition of commutation of differentiation and convolution operators for kernels of this form is satisfied.
Let us consider now case 2, when the plus sign is taken in front of the quadratic term in Eq(13). This case can be interpreted as relaxation of the perturbation arising behind the non-isotropic inclusion when the wave front approaches the next domain. The influence of such a trace of perturbation may turn out to be significant at a sufficiently high concentration of the dispersed phase or domains with various properties (Qiang Du et al., 2018).

$$\frac{d}{d\theta}G_{(k)}(\theta)+Y_{1,(k)}G_{(k)}(\theta)+Y_{2,(k)}G_{(k)}^{2}(\theta)=0\ . \qquad (16)$$

The solution of Eq(16) has the following general form

$$G_{(k)}(\theta)=CY_{1,(k)}\exp\left(-Y_{1,(k)}|\theta|\right)/\left(1-CY_{2,(k)}\exp\left(-Y_{1,(k)}\right)|\theta|\right). \qquad (17)$$

The second spatial scale ought be chosen from the requirement for a faster decrease in the quadratic term in comparison with the linear term with an increase in the distance from the source of disturbance.
From this assumption it follows

$$Y_{1,(k)}=\varphi_{1,(k)}/(\varepsilon^{k}R)\,,Y_{2,(k)}=\varphi_{2,(k)}/(\varepsilon^{2k}R)\ . \qquad (18)$$

Let us consider finally case 3, when the minus sign is taken in front of the quadratic term in Eq(14). This case can be interpreted as description of the emergence and development of a disturbance under substance transfer in inclusive domain in the medium.
The appropriate solution has the following general form

$$G_{(k)}(\theta)=CY_{1,(k)}\exp\left(-Y_{1,(k)}|\theta|\right)/\left(1+CY_{2,(k)}\exp\left(-Y_{1,(k)}\right)|\theta|\right). \qquad (19)$$

Figure 1 depicts the characteristic plots of the relaxation kernels (15), (17), (19).

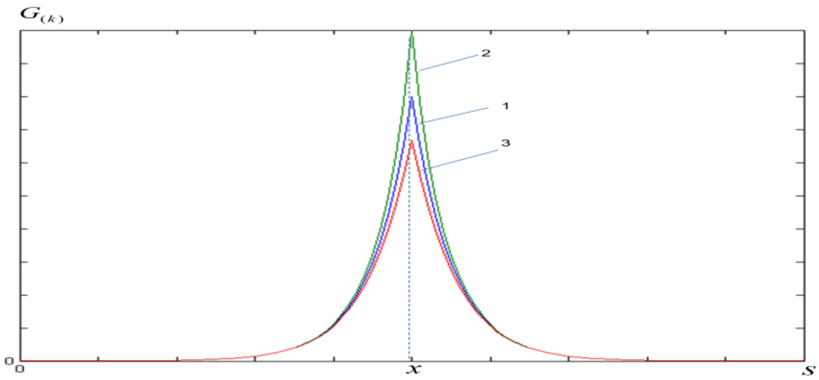

Figure 1: Characteristic plots for the relaxation kernels. 1- Eq(15); 2- Eq(17); 3- Eq(19).

It can be easily proved that condition of commutation of differentiation and convolution operators for kernels of the all considered forms is satisfied. In accordance with the chosen strategy of eliminating the terms of higher than the second order, the following equation can be derived from Eq(8)

$$u_t+\int_{\Omega}G_{(0)}(\theta)u_s ds+2\int_{\Omega}G_{(1)}(\theta)uu_s ds=I\ . \qquad (20)$$

With allowance for the specific behavior of all the considered types of kernels in the integral operators (Figure 1) under a sufficiently fast decrease in $r_{(k)}$ with increasing number k, the following approximation has been substantiated with more correctness

$$\int_{\Omega} G_{(1)}(\theta) u u_s ds \approx \chi \int_{\Omega} G_{(1)}^0(\theta) \delta(x-s) u u_s ds = \chi G_{(1)}^0 u u_x \, , \tag{21}$$

where χ is the normalizing coefficient, $\delta(x-s)$ is the Dirac delta function.
Then, the transfer equation looks as follows

$$u_t + 2\chi G_{(1)}^0 u u_x + \int_{\Omega} G_{(0)}(x-s) u_s ds = I \; . \tag{22}$$

By defining the spatial variable $\varsigma = \dfrac{x}{2\chi G_{(1)}^0}$, the equation can be written as the perturbed Whitham equation.

$$u_t + u u_{\varsigma} + \int_{\Omega} G_{(0)}(\varsigma - s) u_s ds = I \; . \tag{23}$$

With such a rearrangement, the appearances of the kernels (15), (17), (19) do not fundamentally change. At $I = 0$ Eq(24) acquires the form of the usual Whitham equation (Whitham, 1999).

3. Discussion

The solution of Eq(22) can be sought in the form of asymptotic series

$$u = u_0 + \sum_{j=1}^{\infty} \varepsilon^j u_j \; . \tag{24}$$

In order to search for wave solutions, it is advisable to look for the zero term in the form of a single traveling wave

$$u_0 = u_0(\xi). \tag{25}$$

Here $\xi = \varsigma - ct$, c is the phase velocity.
Since Eq(22) has been derived under the weak non-locality assumption in the perturbed form, it would be logical to accept $I = \mathrm{O}(\varepsilon)$. Then, the integration of Eq(22) with respect to the variable ξ in the zero order gives the following result

$$cu_0 - \frac{1}{2} u_0^2 + const = \int_{\Omega} G_{(0)}(\varsigma - s) u_0 ds \; . \tag{26}$$

As the relaxation kernels have a singularity at the point $s = \varsigma$ it is correct to rewrite the integral operator in Eq(26) in the form

$$\int_{\Omega} G_{(0)}(\varsigma - s) u_0 ds = G_{(0)}^0 \left[\int_{-\infty}^{\varsigma} \exp\left(-\frac{\varphi_{(0)}}{r_{(0)}} (\varsigma - s) \right) u_0 ds + \int_{\varsigma}^{\infty} \exp\left(-\frac{\varphi_{(0)}}{r_{(0)}} (s - \varsigma) \right) u_0 ds \right]. \tag{27}$$

Further, after a number of cumbersome, but not complicated in mathematical technique transformations, the following ordinary differential equation has been derived

$$(c - u_0)^2 \frac{d^2 u_0}{d\xi^2} = \frac{\varphi_{(0)} u_0^2}{r_{(0)}} \left[\frac{\varphi_{(0)} u_0^2}{\alpha r_{(0)}} + \left(\beta G_{(0)}^0 - \frac{c\varphi_{(0)}}{2r_{(0)}} \right) u_0 + c \left(\frac{c\varphi_{(0)}}{2r_{(0)}} - G_{(0)}^0 \right) \right], \tag{28}$$

where parameters $\alpha, \; \beta$ are dependent on the type of relaxation function in Eq(11).
Subsequent analysis using the phase plane method shows that equations of such types have solutions in the form of the solitary traveling waves that are capable for propagating over considerable distances with a small change in profile (Newell, 1987).

4. Conclusions

It is shown that the perturbed Whitham equation can be obtained using the nonlinear relaxation function. A wider class of relaxation functions has been considered than it was done before This makes it possible to apply the developed model to describe the propagation of nonlinear waves in heterogeneous media with non-locality at sufficiently high concentrations of the dispersed phase. It was found that for a quadratic relaxation function, it is also possible to reduce the transport equation to the form of a perturbed Whitham equation, which describes the development of nonlinear waves of substance transfer in a reaction medium with nonlocal effects. At the same time, the question of the general form of the kernels of the integral operator in the nonlocal transport law, at which it is possible to reduce the flow equation to the Whitham type remains open. This question should be the subject of further research.

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