Hyperbolicity condition for the hydrodynamical model of charge transport in semiconductor based on Extended Thermodynamics

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Abstract

The condition of hyperbolicity for the hydrodynamical model of semiconductor presented in [1] is investigated. Such a model is based on the Extended thermodynamics and the constitutive closure relations are given up to second order in the deviation from the local partial thermodynamical equilibrium, characterized by zero velocity, heat flux and stress tensor. We will show that the secon order terms considerably enlarge the hyperbolicity region.

1 Introduction

The study of carrier transport in semiconductor devices is of great interest for computer aided design of modern electron devices. An accurate description is given by the model based on a semi-classical kinetic formulation. Their use, however, is not practical because of the large computer times needed for each simulation.

In engineering applications simpler models are routinely used. They give a less detailed description of the system, which is however adequate to describe the gross properties of transport phenomena.

In [2, 3] a hydrodynamical model has been presented in which the closure of the moment equations is obtained from the entropy principle of Extended Thermodynamics [6, 7] (we shall refer to this model as to AP model). Apart from the usual balance equations for carriers density, momentum and energy, the model comprises evolution equations for the heat flux and shear stress. The resulting system is hyperbolic in a suitable domain of the space of variables.

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In this article we investigate the formal properties of an improved version of the extended hydrodynamical model by considering nonlinear closures relations.

These latters are similar to those obtained for a mono atomic non-degenerate gas [8].

Mathematically, the equations have the structure of a quasi-linear hyperbolic system with source. The latter contains a relaxation term and a non local drift term, which is due to a self consistent electric field.

The addition of nonlinear terms in the constitutive relations considerably enlarges the region of hyperbolicity of the model. The main difference is that in the linear model there is a bound on the heat flux, beyond which the system is no longer hyperbolic. In the nonlinear model there is no bound on the heat flux for small viscosity.

The plan of the paper is the following. The basic assumptions are presented in Section 2, and the constitutive relations are outlined in Section 3. Section 4 is devoted to the study of the hyperbolicity conditions of the model.

2 Basic assumptions

In a semi-classical approximation, a kinetic description of the electrons is given by the semi-classical Boltzmann transport equation for the one particle distribution function $f(\mathbf{x}, t, \mathbf{k})$, which represents the probability of finding an electron at time t in an elementary volume $d\mathbf{x}d\mathbf{k}$, around position $\mathbf{x}$ and with crystal momentum $\mathbf{k}$,

$$\frac{\partial f}{\partial t} + v^i(\mathbf{k})\frac{\partial f}{\partial x^i} - eE^i\frac{\partial f}{\partial k^i} = \mathcal{C}[f]. \tag{1}$$

Here e is (the absolute value of) the electron charge, and $\mathbf{k}$ represents the crystal momentum of the electron, belonging to the first Brillouin zone[1] $\mathbf{E}$ is the electric field, and is related to the electron distribution by Poisson's equation:

$$E_i = \frac{\partial \phi}{\partial x_i},$$
$$\epsilon \Delta \phi = -e(N_D - N_A - n),$$

where ϕ is the electric potential, N_D and N_A are respectively the donor and acceptor density, and n is the electron density. The latter is related to f by

$$n = \int f d\mathbf{k}.$$

$\mathcal{C}[f]$ is the collision term, which takes into account scattering with acoustic and optical phonons and with impurities.

The electron velocity $v(\mathbf{k})$ depends on the energy $\mathcal{E}$ measured from the conduction band minimum by the relation

$$v(\mathbf{k}) = \nabla_{\mathbf{k}}\mathcal{E}.$$

In general the band structure may be very complicated, and it depends on the material. In the approximation of a single parabolic conduction band (which we adopt in the rest of the paper),

[1] Einstein summation convention over repeated indices is used, and physical units are such that $\hbar = 1$.

the effective mass is a constant scalar m^*. Then the relation between energy and wave vector and the velocity of the electron are given by

$$\mathcal{E} = \frac{|\mathbf{k}|^2}{2m^*}, \quad v^i = \frac{k^i}{m^*}.$$

Consistently the first Brillouin zone is extended to $\mathbf{R^3}$.

We define the moments of the distribution function f as

$$F_{i_1 i_2 \cdots i_n} = \frac{1}{(m^*)^n} \int d\mathbf{k} f k_{i_1} k_{i_2} \cdots k_{i_n}$$

By multiplying Eq. (1) by $k^{i_1} k^{i_2} \cdots k^{i_n}$ and integrating in $\mathbf{k}$ space, after having employed a suitable vanishing condition for f as $|\mathbf{k}| \to \infty$ in the parabolic band approximation (or in the general case the periodicity condition in the Brillouin zone), one obtains the generic moment equation

$$\frac{\partial}{\partial t} F_{i_1 i_2 \cdots i_n} + \frac{1}{m^*} \frac{\partial}{\partial x^k} F_{i_1 i_2 \cdots i_n k} = Q_{i_1 i_2 \cdots i_n} - eE^i \int d\mathbf{k} \frac{f}{(m^*)^n} \frac{\partial}{\partial k^i} k_{i_1} k_{i_2} \cdots k_{i_n} \tag{2}$$

where $Q_{i_1 i_2 \cdots i_n}$ are the moments of the collision term.

$$Q_{i_1 i_2 \cdots i_n k} = \frac{1}{(m^*)^n} \int d\mathbf{k}\, \mathcal{C}[f] k^{i_1} k^{i_2} \cdots k^{i_n}. \tag{3}$$

The first 13 moments have an immediate physical interpretation:

$$\begin{aligned}
n &= F \quad \text{is the numerical density,} \\
F_i &= \int \frac{d\mathbf{k} f k_i}{(m^*)} \quad \text{is the particle flux,} \\
\frac{1}{2} F_{ii} &= \frac{1}{2} \int \frac{d\mathbf{k} f k^2}{(m^*)^2} \quad \text{is the energy density,} \\
F_{ij} &= \int \frac{d\mathbf{k} f k_i k_j}{(m^*)^2} \quad \text{is the momentum flux density} \\
\frac{1}{2} F_{ill} &= \frac{1}{2} \int \frac{d\mathbf{k} f k_i k^2}{(m^*)^3} \quad \text{is energy flux density}
\end{aligned}$$

and neglecting generation recombination effects, which on the hydrodynamical time scale are negligible, the balance equations in conservation form for the first 13 moments are given[2] the balance equations write in a compact form by

$$\frac{\partial F^A}{\partial t} + \frac{\partial F^{Aj}}{\partial x^j} = P^A. \tag{4}$$

with

$$\begin{aligned}
F^A &= (F, F_i, F_{ll}, F_{<ij>}, F_{ill}), \qquad \mathrm{A} = 1, 2, \cdots, 13 \\
F^{Ak} &= (F_k, F_{ik}, F_{kll}, F_{<ij>k}, F_{ikll}), \\
P^A &= (0, Q^i - \frac{neE_i}{m^*}, Q - \frac{2ne}{m^*} \mathbf{v} \cdot \mathbf{E}, \\
& \quad Q_{<ij>} - \frac{2ne}{m^*} E_{<i} v_{j>}, \hat{Q}_i - \frac{e}{m^*} \left(2F_{il} E^l + F^{ll} E_i \right)),
\end{aligned}$$

[2]Double parenthesis indicate symmetrization. For example for a double tensor, it is $A_{(ij)} = \frac{1}{2}(A_{ij} + A_{ji})$

where Q_i, Q, $Q_{<ij>}$, $\hat{Q}_i$ are the production terms of momentum, energy, deviatoric part of the stress tensor[3], energy flux.

By defining the mean and random component of electron velocity by

$$v_i = \frac{F_i}{n}, \quad k^i = m^*(v^i + c^i),$$

we can introduce the usual thermodynamical variables:

$$\begin{aligned}
\text{the stress tensor} \quad \sigma_{ij} &= m^* \int f c_{<i} c_{j>} d\mathbf{k}, \\
\text{the thermodynamic pressure} \quad p &= n k_B T = \frac{1}{3} \int f c^i c_i d\mathbf{k}, \\
\text{the heat flux} \quad q_i &= \frac{1}{2} \int f c_i c^r c_r d\mathbf{k},
\end{aligned}$$

where T is the electron absolute temperature.

The components of F^A may therefore be rewritten in the more familiar form:

$$\begin{aligned}
F_{ij} &= n v_i v_j + \frac{1}{m^*}(\sigma_{ij} + p\delta_{ij}), \\
F_{ll} &= n v^2 + \frac{3p}{m^*}, \\
F_{ill} &= n v^2 v^i + \frac{1}{m^*}\left(5 p v^i + 2 q^i + 2\sigma_{ij} v^j\right), \\
F_{ijll} &= n v^2 v_i v_j + \frac{1}{m^*}\left[5 \frac{p^2}{n m^*}\delta_{ij} + 3 p v_i v_j + v^2 \sigma_{ij} + p v^2 \delta_{ij} + \right. \\
& \left. 4 v^k v_{(j}(\sigma_{ki)} + p\delta_{ki)}) + 4 v_{(i} q_{j)} + \hat{\theta}_{ijll} + 2\hat{\theta}_{ijr} v_r \right],
\end{aligned}$$

where

$$\hat{\theta}_{ijr} = \frac{m^*}{2} \int d\mathbf{k} f c_i c_j c_r, \quad \hat{\theta}_{ijrs} = \frac{m^*}{2} \int d\mathbf{k} f c_i c_j c_r c_s$$

In order to have a closed system for Eq. (4), it is necessary to express $\hat{\theta}_{ijk}$, $\hat{\theta}_{ijll}$ and productions P^A in terms of F^A.

3 Entropy principle and closure relations

In order to close system (4), in agreement with Extended Thermodynamics, we shall use the entropy principle. One assumes that there exists a supplementary balance law

$$\frac{\partial \eta(F^A)}{\partial t} + \frac{\partial \eta^i(F^A)}{\partial x^i} = g(F^A) \geq 0 \tag{5}$$

which is valid for any solution of system (4). In the previous relation η, η^i and g have the physical meaning of entropy, entropy flux and entropy production.

[3] The deviatoric part of a tensor is the symmetric traceless part of the tensor. For example for a double tensor one has $A_{<ij>} = \frac{1}{2}(A_{ij} + A_{ji}) - \frac{1}{3}A_{ll}\delta_{ij}$

By applying Liu's theorem [5], it is possible to take into account Eq.(5) by introducing the Lagrangian multipliers Λ_A and by solving the inequality

$$\frac{\partial \eta(F^A)}{\partial t} + \frac{\partial \eta^i(F^A)}{\partial x^i} - \sum_A \Lambda_A \left(\frac{\partial F^A}{\partial t} + \frac{\partial F^{Aj}}{\partial x^j} - P^A \right) \geq 0. \tag{6}$$

without constraints. From this inequality it follows

$$\frac{\partial \eta(F^A)}{\partial t} + \frac{\partial \eta^i(F^A)}{\partial x^i} - \sum_A \Lambda_A \left(\frac{\partial F^A}{\partial t} + \frac{\partial F^{Aj}}{\partial x^j} \right) = 0, \tag{7}$$

$$\sum_A \Lambda_A P^A \geq 0. \tag{8}$$

In theory, from Eq.(7) it is possible to derive the constitutive relations. However, the resulting system is highly nonlinear and only in very special cases it is possible to obtain analytical solutions.

In order to obtain analytical results it is therefore necessary to resort to perturbation expansions around local thermodynamical equilibrium, characterized by zero heat flux and viscous stress.

We remark that the situation described here is very different from that arising in gas dynamics. In fact in principle a dependence on the electric field could appear in the lagrangian multipliers. Moreover the field equations are valid only in the frame where the crystal is at rest and the mean electron velocity appearing in the model is the mean elecron velocity with respecy to the crystal. This implies that v^i must be considered as an additional themodynamical variable and the dependence in the fluxes on it cannot be predicted by requiring galilean invariance of the constitutive relations.

To first order in the deviation, one obtains the explicit constitutive relations for $\hat{\theta}_{ijr}$ and $\hat{\theta}_{ijll}$. These imply

$$F_{ijk} = n v_i v_j v_k + \frac{1}{m^*} \left[3 v_{(i} \sigma_{jk)} + 3 p v_{(i} \delta_{jk)} + \frac{6}{5} q_{(i} \delta_{jk)} \right], \tag{9}$$

$$\begin{aligned} F_{ijll} = {} & n v_i v_j v^2 + \frac{1}{m^*} \left[5 \frac{p^2}{n m^*} \delta_{ij} + 3 p v_i v_j + v^2 \sigma_{ij} + p v^2 \delta_{ij} + \right. \\ & \left. \frac{7p}{n m^*} \sigma_{ij} + 4 v^k v_{(j} (\sigma_{ki)} + p \delta_{ki)}) + 4 v_{(i} q_{j)} + \frac{6}{5} q_{(i} \delta_{jk)} v^k \right]. \end{aligned} \tag{10}$$

In the constitutive relations the dependence of the electric field does not appear as shown in [4].

As we shall show in the next section the system obtained by the linear closure is hyperbolic provided the heat flux is suitably bounded.

In order to avoid such limitations one can include other terms in the perturbation expansion around equilibrium. The inclusion of quadratic terms in the expansion will avoid the loss of hyperbolicity for large values of the heat flux.

Monte Carlo data indicate that viscous terms σ_{ij} are always negligible compared to the effects of the heat flux. We shall therefore keep only linear terms in σ_{ij}, and neglect contributions of the form $\sigma_{ik}\sigma^{kj}$ and $\sigma_{ij} q^j$.

To second order in the expansion around equilibrium, Eq. (9) remains unchanged, while (10) becomes [8, 9]

$$\begin{aligned} F_{ijll} &= nv_iv_jv^2 + \frac{1}{m^*}\left[5\frac{p^2}{nm^*}\delta_{ij} + 3pv_iv_j + v^2\sigma_{ij} + pv^2\delta_{ij} + \right. \\ & \left. \frac{7p}{nm^*}\sigma_{ij} + 4v^kv_{(j}(\sigma_{ki)} + p\delta_{ki)}) + 4v_{(i}q_{j)} + \frac{6}{5}q_{(i}\delta_{jk)}v^k + \delta q_iq_j\right]. \end{aligned} \tag{11}$$

The parameter δ cannot be determined from the Liu equations, as in the case of rarefied gas [6].

In order to determine the parameter δ, we resort to a different approach, *the maximum entropy principle*, which under suitable conditions is consistent with Extended Thermodynamics [6].

By applying the maximum entropy principle one obtains

$$\delta = \frac{112}{25p}. \tag{12}$$

This result was independently obtained by in [8] (in the case of gas dynamics) and in [9] (where the more general case of a Fermi electron gas is treated).

It is easy to see that the left hand side of system (7), closed with relations (9)-(10) or (9)-(11) is invariant under Galilean transformations even if such invariance conditions was not required *a priori*.

Now in order to close the system, it is necessary to find constitutive relations for the production terms. These may be obtained by using the maximum entropy distribution function in computing the moments of $\mathcal{C}[f]$. Here we do not discuss these problems (the interested reader can see [1]).

4 Formal properties

The existence of an additional balance law, entropy inequality, has important consequences on the mathematical structure of the field equations.

In fact, if η is a convex function of the field variables, i.e. if the Hessian matrix

$$\left(\frac{\partial^2\eta}{\partial F^A\partial F^B}\right)$$

is positive definite, then the transformation $\Lambda^B = \Lambda^B(F^A)$ is globally invertible. The system, rewritten in terms of the Lagrange multipliers, is symmetric hyperbolic according to Friedrichs and Lax .

In the case of extended thermodynamics, in the approximation of 13 moments, the system that implicitly defines the constitutive equations and the multipliers does not have a known analytical solution. If we make a perturbation expansion around local thermodynamic equilibrium, we obtain an approximate expression of the constitutive equations and the resulting system is not necessarily symmetric hyperbolic. We shall check directly the hyperbolicity of the system, both for linear and nonlinear closures in one dimensional case. Formally, both for the linear and nonlinear closure relations, if we introduce the Jacobian matrix A^0 of density vector F^A, and the Jacobian matrix A^1 of flux vector F^{A1} with respect to the field variables $\mathbf{U} = (n, v, p, \sigma, q)$, the system is written as

$$A^0 \frac{\partial \mathbf{U}}{\partial t} + A^1 \frac{\partial \mathbf{U}}{\partial x} = \mathbf{f}(\mathbf{U}) \tag{13}$$

We recall that system (13) is said hyperbolic if $\det A^0 \neq 0$ and the eigenvalue equation

$$(A^1 - \lambda A^0)\mathbf{r} = 0$$

has real eigenvalues and the eigenvectors span $\mathbf{R}^5$. If the eigenvalues are distinct, the system is said *strictly hyperbolic*.

For $\sigma = q = 0$ it is immediate to see that the system is strictly hyperbolic and the eigenvalues are given by

$$\lambda = v, \quad \lambda = v \pm \sqrt{k_B T (13 \pm \sqrt{94})/m^*}.$$

We expect the system to be hyperbolic in a neighborhood of the region $\sigma = 0$, $q = 0$.

We shall consider separately the linear and nonlinear case.

4.1 Hyperbolicity condition: linear closure

Hyperbolicity conditions for the system with linear closure relations have already been investigated (see [6]). We shall derive them here for completeness.

Since the obtained constitutive equations are invariant under Galilean transformations, if we introduce the convective derivative

$$\frac{d\mathbf{U}}{dt} = \frac{\partial \mathbf{U}}{\partial t} + v \frac{\partial \mathbf{U}}{\partial x},$$

the coefficients of the system

$$\frac{d\mathbf{U}}{dt} + \hat{A} \frac{\partial \mathbf{U}}{\partial x} = \mathbf{f}(\mathbf{U}), \tag{14}$$

with $\hat{A} = (A^0)^{-1} A^1 - v\mathbf{I}$, ($\mathbf{I}$ denotes the 5 by 5 identity matrix), do not depend explicitly on v. Furthermore the eigenvalues $\hat{\lambda}$ of $\hat{A}$ and λ of $(A^0)^{-1} A^1$ are related by $\lambda = v + \hat{\lambda}$.

The characteristic equation

$$det(\hat{A} - \hat{\lambda}\mathbf{I}) = 0, \tag{15}$$

becomes

$$\hat{\lambda} \left[\hat{\lambda}^4 - \left(\frac{26p}{5nm^*} + \frac{62\sigma}{15nm^*} \right) \hat{\lambda}^2 - \frac{96q}{25n(m^*)^{3/2}} \hat{\lambda} + \frac{21\sigma^2}{5(nm^*)^2} \right. \\ \left. + \frac{3p^2}{(nm^*)^2} + \frac{6\sigma p}{(nm^*)^2} \right] = 0. \tag{16}$$

On the boundary of the hyperbolicity region, two of the real roots are coincident, i.e. the characteristic polynomial is of the form

$$\hat{\lambda}(\hat{\lambda}-\hat{\lambda}_1)^2(\hat{\lambda}-\hat{\lambda}_2)(\hat{\lambda}-\hat{\lambda}_3). \tag{17}$$

By comparing (16) with (17), one has

$$\begin{aligned}
\hat{\lambda}_1+\frac{1}{2}(\hat{\lambda}_2+\hat{\lambda}_3) &= 0, && (18)\\
\frac{1}{2}(\hat{\lambda}_2+\hat{\lambda}_3)^2+\frac{1}{4}(\hat{\lambda}_2-\hat{\lambda}_3)^2-\left(\frac{26p}{5nm^*}+\frac{62\sigma}{15nm^*}\right) &= 0, && (19)\\
\frac{21\sigma^2}{5(nm^*)^2}+\frac{3p^2}{(nm^*)^2}+\frac{6\sigma p}{(nm^*)^2}-\frac{1}{4}(\hat{\lambda}_2+\hat{\lambda}_3)^2\hat{\lambda}_2\hat{\lambda}_3 &= 0, && (20)\\
\frac{1}{4}(\hat{\lambda}_2+\hat{\lambda}_3)(\hat{\lambda}_2-\hat{\lambda}_3)^2-\frac{96q}{25n(m^*)^{3/2}} &= 0, && (21)
\end{aligned}$$

By solving the previous system, one obtains that the hyperbolicity region (Fig. 1) is the connected region that contains the origin and is between the two curves

$$\hat{q}=\pm\frac{25}{96}\hat{x}\left(A-\frac{\hat{x}^2}{2}\right), \tag{22}$$

with

$$\hat{x}=\sqrt{2\frac{A+\sqrt{A^2+12C}}{3}}, \quad A=\frac{26}{5}+\frac{62}{15}\hat{\sigma}, \quad C=\frac{21}{5}\hat{\sigma}^2+6\hat{\sigma}+3,$$

where $\hat{q}$ and $\hat{\sigma}$ are the normalized heat flux and shear stress.

$$\hat{q}=\frac{q}{n(k_BT/m^*)^{3/2}}, \quad \hat{\sigma}=\frac{\sigma m^*}{nk_BT}.$$

4.2 Hyperbolicity conditions: nonlinear closure

The characteristic polynomial in the nonlinear case becomes

$$\begin{aligned}
&\lambda\left[\lambda^4-\frac{148}{25}\frac{q}{p\sqrt{m^*}}\lambda^3+\left(\frac{148}{75}\frac{q^2}{p^2}-\frac{62}{15}\frac{\sigma}{n}-\frac{26}{5}\frac{p}{n}\right)\frac{\lambda^2}{m^*}\right.\\
&\left.+\left(\frac{444}{25}\frac{\sigma q}{pn}+\frac{348}{25}\frac{q}{n}\right)\frac{\lambda}{(m^*)^{3/2}}+\frac{1}{(m^*)^2}\left(\frac{21}{5}\frac{\sigma^2}{n^2}-\frac{444}{125}\frac{\sigma q^2}{p^2 n}+6\frac{\sigma p}{n^2}+3\frac{p^2}{n^2}\right)\right].
\end{aligned} \tag{23}$$

With an obvious notation, we rewrite it in the form

$$\lambda\left[\lambda^4+a\lambda^3+b\lambda^2+c\lambda+d\right], \tag{24}$$

and introduce the affine transformation

$$\lambda=\left(z-\frac{a}{4}\right).$$

The characteristic equation becomes

$$\left(z - \frac{a}{4}\right)\left[z^4 + \left(b - \frac{3}{8}a^2\right)z^2 + \left(\frac{1}{8}a^3 + c - \frac{1}{2}ab\right)z - \frac{3}{256}a^4 + d - \frac{1}{4}ac + \frac{a^2 b}{16}\right] = 0. \tag{25}$$

The situation is therefore similar to the case of the linear closure.

By letting

$$A = \frac{3}{8}\hat{a}^2 - \hat{b}, \quad B = \frac{\hat{a}\hat{b}}{2} - \frac{\hat{a}^3}{8} - \hat{c}, \quad C = -\frac{3}{256}\hat{a}^4 + \hat{d} - \frac{\hat{a}\hat{c}}{4} + \frac{\hat{a}^2\hat{b}}{16},$$

with

$$\begin{aligned} \hat{a} &= -\frac{148}{25}\hat{q}, \quad \hat{b} = \frac{148}{75}\hat{q}^2 - \frac{62}{15}\hat{\sigma} - \frac{26}{5}, \\ \hat{c} &= \frac{444}{25}\hat{\sigma}\hat{q} + \frac{348}{25}\hat{q}, \quad \hat{d} = \frac{21}{5}\hat{\sigma}^2 - \frac{444}{125}\hat{\sigma}\hat{q}^2 + 6\hat{\sigma} + 3, \end{aligned}$$

one obtains that the hyperbolicity region is the connected one that contains the origin and that lies between the two curves implicitly defined by the equations

$$B = \pm\hat{x}\left(A - \frac{\hat{x}^2}{2}\right), \quad \text{with} \quad \hat{x} = \sqrt{\frac{2}{3}\left(A + \sqrt{A^2 + 12C}\right)}.$$

Fig. 1 shows the hyperbolicity region both in the linear and nonlinear case. The hyperbolicity region in the nonlinear case is broader than the one corresponding to the linear closure. Furthermore we observe that for small values of the shear stress there are no limitations on the heat flux. Because viscosity is usually negligible, the inclusion of nonlinear terms in practice guarantees the hyperbolicity of the model in the cases which are relevant for the applications.

Acknowledgments

This work has been partially supported by MURST, and by CNR project *Modelli matematici per semiconduttori. Progetto speciale: metodi matematici in fluidodinamica e dinamica molecolare*, grant number 96.03855.CT01.

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Figure captions

Fig. 1. The connected region containing the origin and bounded by the dashed line represents the region of hyperbolicity for the model with the linear closure. The connected region containing the origin and bounded by the continuous line represents the region of hyperbolicity for the model with the nonlinear closure. The inclusion of the quadratic terms in the constitutive equations enlarges considerably the region of hyperbolicity.