Extended Hydrodynamical Model of Carrier Transport in Semiconductors

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Abstract

A hydrodynamical model based on the theory of Extended Thermodynamics is presented for carrier transport in semiconductors. Closure relations for fluxes are obtained by employing the maximum entropy principle. The production terms are modeled by means of a fitting of the Monte Carlo data for homogeneously doped semiconductors.

The mathematical properties of the model are studied. A suitable numerical method, which is a generalization of the Nessyahu-Tadmor scheme to the non homogeneous case, is provided.

The validity of the constitutive relations has been assessed by comparing the numerical results with detailed Monte Carlo simulations.

Keywords: semiconductors, hydrodynamical model for charge transport, hyperbolic systems, shock-capturing numerical methods for conservation laws.

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1 Introduction

The study of carrier transport in semiconductor devices is of great interest for the design of modern electron devices. Detailed Monte Carlo simulations are based on a semi-classical kinetic formulation, and provide an accurate description of charge transport in sub-micron devices [1, 2]. Their use, however, is not practical for Computer Aided Design, 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.

Among these models, the more commonly used ones are the *Drift -Diffusion* model [3, 4, 5], their extensions including the carrier energy (called energy models) [1, 3, 7, 8], and hydrodynamic models [3, 6]. The Drift-Diffusion and energy models can be derived formally by a Chapman-Enskog type expansion of the transport equation [9, 10] and thermodynamically from linear irreversible thermodynamics [7]. They give satisfactory answers for device sizes of the order of a few microns and moderate applied voltages, because in this case the assumption of local thermodynamical equilibrium is a reasonable approximation. The energy model essentially comprises the balance equations for the carrier density end energy density, supplemented by linear constitutive laws relating the particle and energy fluxes to the gradient of chemical potential and energy density. For submicron devices high field effects must be taken into account and linear relations are no longer valid as showed for instance by the loss of validity of the Onsager reciprocity relations for fields exceeding about 10^4 V/cm [15]. Hydrodynamic models aim to provide a description of such non equilibrium effects without the overhead of large computational costs typical of kinetic models.

Among the various hydrodynamical models, the one introduced by Blotekjaer [6] and subsequently thoroughly investigated by Baccarani and coworkers [12] (which we shall denote by BBW), is incorporated in several commercial simulation packages. It comprises the balance equations for carriers density, momentum and energy, obtained as moment equations of the underlying kinetic Boltzmann transport equation. The closure of the moment equations is achieved by postulating a phenomenological constitutive relation of Fourier type for the heat flux. Thermal conductivity contains a free parameter, whose value is chosen *ad hoc* by comparison with Monte Carlo results [11].

Numerical simulations indicate, however, that the adopted expression of the heat flux is not in qualitative agreement with Monte Carlo results (see for example [13, 14]). Furthermore, the Onsager reciprocity relations are not satisfied [15] in this model.

A more accurate hydrodynamical model has been recently developed by Tang and coworkers [14]. They determine the constitutive relations with a calibration of the free parameters from MC data without imposing *a priori* a Fourier law for the heat flux and by considering the energy flux as an additional independent dynamical variable. This model can be very useful for problems such as stability analysis, which is more easily performed in a hydrodynamical context, but it is heavily dependent on MC results. It is therefore desirable to have constitutive relations of general validity obtained on the basis of fundamental physical laws.

In this sense a considerable improvement on the BBW model has been introduced by Anile and Pennisi [16], in which the closure of the moment equations is obtained from the entropy principle of Extended Thermodynamics [20, 21] (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. In the stationary case, by linearizing the heat flux equation for small temperature gradients (Maxwellian iteration) one obtains an extension of the Fourier law which includes also a convective term. With the addition of this term, the Onsager relations for small deviations from thermodynamical equilibrium are restored. Furthermore the heat conductivity turns out to be directly related to the energy-flux relaxation time and does not contain any undetermined free parameters.

In [25] a numerical scheme has been presented for the numerical solution of the BBW and AP equations for 1D non stationary problems. The equations contain a hyperbolic term and a term representing diffusive, relaxation and drift effects. A splitting technique has been used. The convection step takes care of the hyperbolic part, while the other effects are treated in a second step (relaxation step). The hyperbolic step has been solved by the scheme proposed by Nessyahu and Tadmor (NT) [26], which has the advantage over upwind-based schemes that it does not require the knowledge of the characteristic speeds of the system. This property is crucial in the case of the AP model, since in this case there is no simple explicit expression for the eigenvalues of the hyperbolic part of the system. This instead is the case for the BBW model, whose hyperbolic part coincides with the Euler hydrodynamical equations and for which shock capturing schemes can be naturally adopted [27, 28]. The numerical results have been compared with those obtained by the Monte Carlo code DAMOCLES [2, 29].

The AP model gives a better prediction for the heat flux than the BBW model, but the results for velocity and energy are not fully satisfactory.

In this article we investigate an improved version of the extended hydrodynamical model previously introduced by Anile and Muscato [15], by considering also nonlinear closures and a more accurate representation for the production terms. In the previous formulation the closure relation for the deviatoric part of the flux of energy flux was a linear one, i.e. it contained up to terms of first order in the deviation off a suitably defined state of local thermal equilibrium. The explicit form for the linear constitutive relation was explicitly obtained from the entropy principle [16, 20]. However, the method based on the entropy principle was not able to determine all the coefficients of the second order corrections. The undetermined coefficients, however can be obtained by an application of the *maximum entropy approach* [30, 33, 37]. The explicit results for non-degenerate gas has been obtained in [34, 35].

However in the case of semiconductors some differences arise because a full description involves a mixture of electron, hole and phonon gases. In the applications it is often a reasonable approximation to neglect the motion of the hole and consider the crystal as a thermal bath. Therefore a natural privileged frame there exists to observe the motion of the charge carriers: the rest frame of the crystal. As a consequence the electron velocity appears as relative velocity and must be considered, in order to determine the constitutive equations, as an effective thermodynamical variable.

The relaxation times have been obtained with a fitting of the MC data in the homogeneous case on the base of representation formulas for tensor-valued functions.

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. We have investigated this system for the case of a 1D quasi-ballistic $n^+ - n - n^+$ diode, which is a sort of *benchmark* problem for models of sub-micron electron devices.

The numerical results have been compared with Monte Carlo simulations and a good agreement is observed in the field variables for realistic lengths of the channel.

The plan of the paper is the following. The basic assumptions are presented in Section 2, and the constitutive relations are outlined in Sections 3 and 4. Section 5 is devoted to the study of the formal properties of the model. In the last two sections we recall the computational scheme and show the numerical results.

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 $\mathbf{k}$ [4],

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

Similar equations should be included for holes and phonons (these latters account for the energy transport inside the lattice). In the sequel we neglect the motion of holes and consider the crystal as a thermal bath at constant temperature T_0. Thereafter all the relations will be understood to hold in the rest frame of the crystal.

In (1) 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

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

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 (see [36]). Its expression is of the form:

$$\mathcal{C}[f] = \int d\mathbf{k}' \left[s(\mathbf{x}, \mathbf{k}', \mathbf{k}) f'(1-f) - s(\mathbf{x}, \mathbf{k}, \mathbf{k}') f(1-f') \right]. \tag{2}$$

The first term gives the total probability that an electron at $\mathbf{x}$ with momentum $\mathbf{k}'$ is scattered to the state $(\mathbf{x}, \mathbf{k})$, while the second term gives the total probability that an electron in $(\mathbf{x}, \mathbf{k})$ is scattered to $(\mathbf{x}, \mathbf{k}')$. The terms $1-f$ and $1-f'$ describe the effect of the Pauli exclusion principle. Note that the distribution function f is normalized in such a way that it represents the occupation probability of the quantum state denoted by the wave vector $\mathbf{k}$. This normalization is justified also in the semi-classical approach. In fact, if the distribution function represents a probability at the initial time (i.e. if $0 \leq f(x, k, 0) \leq 1$), then this bound is maintained by the solution of the transport equation (1),(2) for later times $(0 \leq f(x, k, t) \leq 1)$ [4].

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

$$u^i(\mathbf{k}) = \nabla_{k^i} \mathcal{E}.$$

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), the effective mass is a constant scalar m^*, and the relation between energy and wave vector is

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

and therefore

$$u^i = \frac{k^i}{m^*}.$$

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

Equation (1) is a nonlinear integro-differential equation in 7 independent variables. Simpler approximate models can be derived from the kinetic equation.

The main approximations are based on the expansion of the distribution function around the Maxwell-Boltzmann equilibrium distribution (e.g. Drift-Diffusion model), and the moment method (hydrodynamic models). The latter are introduced as follows. We define the moments of the distribution function f,

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

By multiplying Eq. (1) by $k^{i_1} k^{i_2} \cdots k^{i_n}/(m^*)^n$ 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

$$\frac{\partial}{\partial t} F_{i_1 i_2 \cdots i_n} + \frac{1}{m^*} \frac{\partial}{\partial x^k} F_{i_1 i_2 \cdots i_n k} = Q_{i_1 i_2 \cdots i_n} - eE^i \int d\mathbf{k} \frac{f}{(m^*)^n} \frac{\partial}{\partial k^i} k_{i_1} k_{i_2} \cdots k_{i_n} \tag{3}$$

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

$$Q_{i_1 i_2 \cdots i_n k} = \frac{1}{(m^*)^n} \int d\mathbf{k}\, \mathcal{C}[f] k^{i_1} k^{i_2} \cdots k^{i_n}. \tag{4}$$

In this way there are only four independent variables, but the system is infinite, because the first N equations comprise the first $N+1$ moments. An approximate system is obtained by a suitable truncation of the hierarchy. This procedure can be used at different levels. We shall take into account models whose moments have an immediate physical interpretation. Let us consider the first moments:

numerical density $\quad n = F,$

particle flux $\quad F_i = \int f u_i \, d\mathbf{k},$

energy density $\quad \frac{1}{2} F_{ii} = \frac{1}{2} \int f u^2 \, d\mathbf{k},$

momentum flux density $\quad F_{ij} = \int f u_i u_j \, d\mathbf{k},$

energy flux density $\quad \frac{1}{2} F_{ill} = \frac{1}{2} \int f u_i u^2 \, d\mathbf{k}$

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 by[2]

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial x^k} F_k = 0, \tag{5}$$

$$\frac{\partial F_i}{\partial t} + \frac{\partial}{\partial x^k} F_{ik} = Q_i - \frac{neE_i}{m^*}, \tag{6}$$

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

$$\begin{aligned}
\frac{\partial F_{ll}}{\partial t} + \frac{\partial}{\partial x^k} F_{llk} &= Q - \frac{2ne}{m^*}\mathbf{v}\cdot\mathbf{E}, && (7)\\
\frac{\partial F_{<ij>}}{\partial t} + \frac{\partial}{\partial x^k} F_{<ij>k} &= Q_{<ij>} - \frac{2ne}{m^*}E_{<i}v_{j>}, && (8)\\
\frac{\partial F_{ill}}{\partial t} + \frac{\partial}{\partial x^k} F_{ikll} &= \hat{Q}_i - \frac{e}{m^*}\left(2F_{il}E^l + F^{ll}E_i\right), && (9)
\end{aligned}$$

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 introducing the notation

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

the balance equations write in a compact form

$$\frac{\partial F^A}{\partial t} + \frac{\partial F^{Aj}}{\partial x^j} = P^A. \qquad (10)$$

We remark that the balance equations have not been postulated or based on general principles of continuum mechanics, but they have been derived as moment equations of the transport equations for electrons.

By defining the mean and random component of electron relative velocity by

$$k^i = m^* u^i = m^*(v^i + c^i),$$

we can introduce the usual thermodynamical variables:

stress tensor $\quad \sigma_{ij} = m^* \int f c_{<i}c_{j>}\, d\mathbf{k}$,

thermodynamic pressure $\quad p = nm^* k_B T = \frac{1}{3} m^* \int f c^i c_i \, d\mathbf{k}$,

heat flux $\quad q_i = \frac{1}{2} m^* \int f c_i c^r c_r \, d\mathbf{k}$,

where T is the electron absolute temperature.

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

$$\begin{aligned}
F_{ij} &= nv_iv_j + \frac{1}{m^*}(\sigma_{ij} + p\delta_{ij}), && (11)\\
F_{ll} &= nv^2 + \frac{3p}{m^*}, && (12)\\
F_{ill} &= nv^2v^i + \frac{1}{m^*}\left(5pv^i + 2q^i + 2\sigma_{ij}v^j\right), && (13)\\
F_{ijll} &= nv^2v_iv_j + \frac{1}{m^*}\left[3pv_iv_j + v^2\sigma_{ij} + pv^2\delta_{ij} + \right. && (14)\\
&\quad \left. 4v^k v_{(j}(\sigma_{ki)} + p\delta_{ki)}) + 4v_{(i}q_{j)} + \hat{\theta}_{ijll} + 2\hat{\theta}_{ijr}v_r\right], && (15)
\end{aligned}$$

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

where

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

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

In order to have a closed system for Eq. (10), it is necessary to express $\hat{\theta}_{ijk}$, $\hat{\theta}_{ijll}$ and productions P^A in terms of F^A.

It is important to stress that, at variance of the monoatomic gas, here the $\hat{\theta}_{ijk}$, $\hat{\theta}_{ijll}$ and productions P^A can depend also on the relative velocity and such dependence cannot be determined by resorting to Galilean invariance because the frame is comoving with the crystal.

3 Maximum entropy principle and closure relations for fluxes

In order to close system (10), in agreement with the information theory and molecular extended thermodynamics [30, 37, 20, 21] we shall use the maximum entropy principle (MEP). This latter states that if a certain number of moments are known one can evaluate the unknown moments by mean of the distribution f_{ME} which makes stationary the entropy functional under the constraints that it yields exactly the known moments. Then one can use the f_{ME} to evaluate the unknown quantities presented in the balance equations as functions of the moments assumed as fundamental variables. Another advantage of considering the maximum entropy principle is that it gives a first guess of the exact distribution function and therefore it can be useful in the implementation of hybrid numerical code, where in the rarefied regime the transport equation is solved while in the fluid regime the macroscopic balance equation are considered. However we want to stress that a general result relating the solution of the transport equation and the distribution function obtained by employing the MEP does not exist. In the present paper we shall use f_{ME} only to the aim to have a reasonable and physically sound way to find the closure relations for the balance equations.

Our system of electron gas and thermal bath of lattice impurities and phonons obeys a Maxwell-Boltzmann statistics with the following entropy functional [31, 32] which ensures a positive entropy production for the Boltzmann-Poisson system

$$s = -k_B \int_{\mathcal{R}^3} \left(f \log f - f + \frac{m^* u^2}{2 k_B T_0} f \right) d^3\mathbf{k}. \tag{16}$$

Therefore we have to find the extremal f_{ME} of the functional s under the constraints

$$F_A = \int_{\mathcal{R}^3} \psi_A f_{ME} d^3\mathbf{k}, \tag{17}$$

with

$$\psi_A = \left(1,\, u^i,\, u_{<i}u_{j>},\, \frac{1}{2}u_l u^l,\, \frac{1}{2}u^i u_l u^l\right),$$

u^i being the particle velocity $u^i = k^i/m^*$.

It is customary to introduce the Lagrangian multipliers Λ_A and the Legendre transformation of s,

$$s' = s - \Lambda_A F^A,$$

and maximize s' without constraints.

From the conditions

$$\delta s' = 0,$$

one has

$$f_{ME} = \exp\left[-\frac{m^* u^2}{2k_B T_0} - \Lambda_A \psi^A\right],$$

that is

$$f_{ME} = \exp\left[-\left(\lambda + u_i\lambda^i + \frac{1}{2}u_l u^l \lambda_{rr} + u^{<i}u^{j>}\lambda_{<ij>} + \frac{1}{2}u^i u_l u^l \lambda_{irr}\right)\right], \qquad (18)$$

where λ, λ^i, $\lambda_{<ij>}$ and λ_{ill} are the Lagrangian multipliers relative to the number density, the velocity, the energy, the stress tensor and the energy flux respectively, while $\lambda_{ll} = \lambda_{ll}^{(el)} + 1/k_B T_0$ is the Lagrangian multiplier relative to the energy. This latter is the sum of a term due to the electron, $\lambda_{ll}^{(el)}$, and a term due to the crystal, $1/k_B T_0$.

Monte Carlo simulations for electron transport in silicon show that the distribution function is almost isotropic. Therefore we shall assume that

$$f_{ME} = \exp\left\{-\left[\lambda + \frac{1}{2}u_l u^l \lambda_{rr} + \delta\left(u_i\lambda^i + u^{<i}u^{j>}\lambda_{<ij>} + \frac{1}{2}u^i u_l u^l \lambda_{irr}\right)\right]\right\}, \qquad (19)$$

with δ a formal *small* parameter. By expanding up to second order in δ,

$$f_{ME} = \exp\left[-\left(\lambda + \frac{1}{2}u_l u^l \lambda_{rr}\right)\right](1 - \delta x + \delta^2 \frac{x^2}{2}) + o(\delta^2), \qquad (20)$$

where

$$x = u_i\lambda^i + u^{<i}u^{j>}\lambda_{<ij>} + \frac{1}{2}u^i u_l u^l \lambda_{irr}.$$

We remark that the distribution (20) is integrable on $\mathbf{R^3}$.

Now in order to express f_{ME} as functions of the moments F_A, we must express the Lagrangian multipliers in terms of the F_A by inverting the following algebraic nonlinear system

$$n = \int \frac{d\mathbf{k} f_{ME} k_i}{(m^*)}, \qquad (21)$$

$$F_i = \int \frac{d\mathbf{k} f_{ME} k_i}{(m^*)}, \qquad (22)$$

$$
\begin{aligned}
\frac{1}{2}F_{ii} &= \frac{1}{2}\int \frac{d\mathbf{k} f_{ME} k^2}{(m^*)^2}, && (23)\\
F_{<ij>} &= \int \frac{d\mathbf{k} f_{ME} k_i k_j}{(m^*)^2}, && (24)\\
\frac{1}{2}F_{ill} &= \frac{1}{2}\int \frac{d\mathbf{k} f k_i k^2}{(m^*)^3} && (25)
\end{aligned}
$$

We assume that the multipliers are analytic function of δ and by the representation formulas for isotropic functions one has

$$
\begin{aligned}
\lambda &= \lambda^{(0)} + \delta^2\lambda^{(2)} + o(\delta^2), && (26)\\
\lambda_i &= \delta\lambda_i^{(1)} + \delta^2\lambda_i^{(2)} + o(\delta^2) && (27)\\
\lambda_{rr} &= \lambda_{rr}^{(0)} + \delta^2\lambda_{rr}^{(2)} + o(\delta^2), && (28)\\
\lambda_{<ij>} &= \delta\lambda_{<ij>}^{(2)} + \delta^2\lambda_{<ij>}^{(2)} + o(\delta^2), && (29)\\
\lambda_{irr} &= \delta\lambda_{irr}^{(1)} + \delta^2\lambda_{irr}^{(2)} + o(\delta^2). && (30)
\end{aligned}
$$

If the previous expression of the multipliers are inserted into the relations (21)-(25), by taking into account the following formula valid for $\mathbf{l}$ belonging to S^2, the unit sphere of $\mathbf{R^3}$,

$$
\int_{S^2} l^{i_1}\cdots l^{i_k}\, d\Omega = \begin{cases} 0 & \text{if } k \text{ is odd} \\ \frac{4\pi}{k+1}\delta^{(i_1 i_2}\delta^{i_3 i_4}\cdots\delta^{i_{k-1} i_k)} & \text{if } k \text{ is even} \end{cases},
$$

where $\delta^{(ij}$ denotes the Kronecker delta, and the formula (for a, $\nu > 0$)

$$
\int_0^\infty x^{\nu-1}\exp(-ax)\,dx = \frac{1}{a^\nu}\Gamma(\nu),
$$

with $\Gamma(\nu)$ the special Gamma function, and the property valid for positive integers p

$$
\Gamma\left(p + \frac{1}{2}\right) = \frac{\sqrt{\pi}}{2^p}(2p-1)!!,
$$

after tedious but simple calculations one finds the Lagrangian multipliers as functions of the moments F_A.

If for the F_A we use the decomposition (11)-(15), the following explicit expressions are obtained

$$
\begin{aligned}
\lambda &= -\log\frac{n(m^*)^2}{(2\pi m^* k_B T)^{3/2}} + \frac{m^*\mathbf{v}\cdot\mathbf{v}}{2k_B T} - \frac{m^*}{n(k_B T)^2}\mathbf{v}\cdot\mathbf{q} - \frac{2}{5}\frac{m^*}{n^2(k_B T)^3}\mathbf{q}\cdot\mathbf{q}\\
&\quad -\frac{1}{4}\frac{\sigma_{kr}\sigma_{kr}}{n^2(k_B T)^2},\\
\lambda_{rr} &= \frac{1}{k_B T} + \frac{2}{3}\frac{m^*\mathbf{v}\cdot\mathbf{q}}{n(k_B T)^3} + \frac{2}{5}\frac{m^*\mathbf{q}\cdot\mathbf{q}}{n^2(k_B T)^4} + \frac{1}{3}\frac{\sigma_{kr}\sigma_{kr}}{n^2(k_B T)^3},\\
\lambda_i &= -\frac{m^*}{k_B T}v_i + \frac{m^*}{n(k_B T)^2}q_i + \frac{m^*\sigma_{ij}v^j}{n(k_B T)^2} - \frac{7}{5}\frac{m^*\sigma_{ij}q^j}{n^2(k_B T)^3},
\end{aligned}
$$

$$\lambda_{<ij>} = -\frac{1}{2}\frac{\sigma_{ij}}{n(k_BT)^2} + \frac{2}{5}\frac{m^*}{n(k_BT)^3}v_{<i}q_{j>} + \frac{9}{25}\frac{m^*}{n^2(k_BT)^4}q_{<i}q_{j>} + \frac{1}{2}\frac{\sigma_{<ir}\sigma_{rj>}}{n^2(k_BT)^3},$$
$$\lambda_{irr} = -\frac{2}{5}\frac{m^*}{n(k_BT)^3}q_i + \frac{18}{25}\frac{m^*}{n^2(k_BT)^4}\sigma_{ij}q^j.$$

They are the *same* of those obtained in [34] for monoatomic gas, although the velocity here plays a different role.

Similar results were found in [33] in the case of a Fermi electron gas by introducing the decomposition of the Lagrangian multipliers into convective and non-convective parts, by imposing the condition that the non-convective parts are independent on the velocity and by performing an expansion around a state of partial thermodynamic equilibrium (whose meaning is not totally clear at kinetic level because it involves the presence of different time scales which are not evident from the expression of the distribution function, but can be obtained by analyzing the collision operator only after the expression of f_{ME} has been obtained).

This procedure followed in [33] has been justified on the basis of the properties proved in [18] according to which the entropy production is an objective quantity if and only if the non-convective part are independent on the velocity. Such a result was obtained by using the method of Liu [19] while our derivation has been performed coherently in the framework of the molecular extended thermodynamics by imposing conditions only on the form of the distribution function and without resorting to the ambiguous concept of state of partial thermodynamical equilibrium.

For $\hat{\theta}_{ijr}$ and $\hat{\theta}_{ijll}$ we get the following expressions

$$\hat{\theta}_{ijr} = \frac{12}{5pm^*}q_{<i}\sigma_{jr>} + \frac{6}{5m^*}q_{(i}\delta_{jr)}, \tag{31}$$
$$\hat{\theta}_{ijll} = \frac{5p^2}{n(m^*)^2}\delta_{ij} + \frac{7p}{n(m^*)^2}\sigma_{ij} + \frac{2}{n(m^*)^2}\sigma_{ik}\sigma_{kj} + \frac{112}{25p(m^*)^2}q_iq_j + \frac{36}{25}\frac{q^2}{p(m^*)^2}\delta_{ij}. \tag{32}$$

These imply

$$F_{ijk} = nv_iv_jv_k + \frac{1}{m^*}\left[3v_{(i}\sigma_{jk)} + 3pv_{(i}\delta_{jk)} + \frac{6}{5}q_{(i}\delta_{jk)} + \frac{12}{5p}q_{<i}\sigma_{jk>}\right], \tag{33}$$
$$\begin{aligned} F_{ijll} = {} & nv_iv_jv^2 + \frac{1}{m^*}\Big[5\frac{p^2}{nm^*}\delta_{ij} + 3pv_iv_j + v^2\sigma_{ij} + pv^2\delta_{ij} + \\ & \frac{7p}{nm^*}\sigma_{ij} + 4v^kv_{(j}(\sigma_{ki)} + p\delta_{ki)}) + 4v_{(i}q_{j)} + \frac{12}{5}q_{(i}\delta_{jk)}v^k \\ & + \frac{2}{nm^*}\sigma_{ik}\sigma_{kj} + \frac{112}{25pm^*}q_iq_j + \frac{24}{5pm^*}q_{<i}\sigma_{jk>}v^k + \frac{36}{25}\frac{q^2}{pm^*}\delta_{ij}\Big]. \end{aligned} \tag{34}$$

We remark that in our model the velocity is a first order quantity. Consistently with the quadratic expansion, in the expressions for F_{jk} and F_{ijll} higher order terms in the velocity are neglected. This expansion is therefore more consistent than the one presented in [16, 15, 33].

Moreover Monte Carlo data indicate that viscous terms σ_{ij} are always negligible compared to the effects of the heat flux. Indeed it is quite standard in the existing literature on hydrodynamical models for semiconductors consider the electron gas as inviscid. We shall keep only linear terms in σ_{ij} and neglect contributions of the form $\sigma_{ik}\sigma^{kj}$, $\sigma_{ij}q^j$ and $\sigma_{ij}vj$.

Therefore the final form of the closure relations for fluxes is

$$F_{ijk} = \frac{1}{m^*}\left[3pv_{(i}\delta_{jk)} + \frac{6}{5}q_{(i}\delta_{jk)}\right], \tag{35}$$

$$\begin{aligned} F_{ijll} &= \frac{1}{m^*}\left[5\frac{p^2}{nm^*}\delta_{ij} + 3pv_iv_j + pv^2\delta_{ij} + \frac{7p}{nm^*}\sigma_{ij} + 4v^k v_{(j}p\delta_{ki)}\right. \\ &\left. +4v_{(i}q_{j)} + \frac{12}{5}q_{(i}\delta_{jk)}v^k + \frac{112}{25pm^*}q_iq_j + \frac{36}{25}\frac{q^2}{pm^*}\delta_{ij}\right]. \end{aligned} \tag{36}$$

4 Closure relations for the production terms

Now in order to close the system, it is necessary to find constitutive relations for the production terms. These may be obtained by using again the distribution function obtained with the maximum entropy principle. However, because of the difficulty of the problem, no satisfactory analytical approximation has been obtained so far. Furthermore, as it has been observed in [30] in the case of rarefied gases, because of the truncation of the moment expansion of the density function f to finite order, the procedure applied to the collision operator might lead, for the transport parameter, to rather large discrepancy with MC simulations. We therefore follow another approach in modeling the production terms.

In the framework of a hydrodynamical model we assume that the productions are functions of the fields F^A. In gas dynamics the requirement of Galilean invariance determines the general expression for Q^A. In the case of carrier transport in semiconductors such expressions cannot be used.

The representation theorems show that the productions Q_i and $\tilde{Q}_i$ have the general form

$$Q_i = d_1F_i + d_2S_i + d_3F_{ij}F^i + d_4F_{ij}S^j + \cdots \tag{37}$$

and similarly for $\tilde{Q}_i$, with $S_i = \frac{1}{2}F_{ill}$. The coefficients d_i are functions of the independent scalar quantities that can be obtained with the F^A's, e.g. F^iF_i, $F^i_kF^i_k$ and so on.

However if we restrict our attention to the case of silicon semiconductors, the scattering are isotropic [36] and we can retain only the first two terms in the expansion (37). This is also consistent with a quadratic modeling of the closure relations.

The same considerations lead to the following expression for $Q_{<ij>}$

$$Q_{<ij>} = -d\frac{F_{<ij>}}{m^*}. \tag{38}$$

The coefficient d is the inverse of the viscosity relaxation time,

$$d = \frac{1}{\tau_\sigma}.$$

Now let us consider the production of the energy balance equation. Since Q is a scalar quantity, expansion (37), together with the isotropy assumption, leads to a term of the form:

$$Q = -2\frac{W - W_0}{m^* \tau_W}, \tag{39}$$

with $W = \frac{1}{2}F_{ll}$ and $W_0 = \frac{3}{2}nk_B T_0$, T_0 being the lattice temperature, and τ_W denotes the energy relaxation time.

The relaxation times τ_W, τ_σ are, like the coefficients d_i, function of the scalar quantities that can be constructed with the F^A. Moreover, all the transport coefficients may depend on the doping concentration (if scattering with the impurities is considered).

The above constitutive laws for the productions are local. Therefore they must have the same expression both in the homogeneous and non-homogeneous case. This enables us to determine the transport coefficients from the MC data obtained for homogeneous doped silicon [15].

The energy relaxation time is obtained by fitting the MC data with the functional form

$$\tau_W = a_1 + a_2 r + a_3 \exp(-a_4 r)$$

where $r = W/W_0 - 1$, $W_0 = \frac{3}{2}k_B T_0$. We obtain the following values for the coefficients

$$\mathbf{a} = [0.4012, 0.0126, 1.0387, 1.8734],$$

with the a_i expressed in picosecond. However for the application τ_W can be considered constant (relevant deviations are only for energy lower than 0.05 eV). The more appropriate value is $\tau_W = 0.47$ ps.

For the analysis of Q_i and $\tilde{Q}_i$, in the one dimensional case it is more useful to introduce the relaxation time of momentum τ_p and energy flux τ_q, defined according to

$$Q_1 = -\frac{J}{\tau_p}, \tag{40}$$

$$\tilde{Q}_1 = -\frac{2S}{\tau_q} \tag{41}$$

where J and S are the components of F_i and $1/2F_{ill}$ along the direction of motion.

As previously observed in [14], τ_p^{-1} and τ_q^{-1} are single-valued functions of the ratio S/J. But at variance with [14] we use a quadratic function to fit the MC results

$$\tau_p^{-1} = c_1 + c_2\frac{S}{J} + c_3\frac{S^2}{J^2}, \tag{42}$$

$$\tau_q^{-1} = \tilde{c}_1 + \tilde{c}_2\frac{S}{J} + \tilde{c}_3\frac{S^2}{J^2}. \tag{43}$$

The values of the c_i and $\tilde{c}_i$ are the following:

$$\begin{aligned}
c_1 &= 0.32 \quad \mathrm{ps}^{-1}, \\
c_2 &= 77.586 \quad \mathrm{ps}^{-1}\mathrm{eV}^{-1}, \\
c_3 &= \text{-}80.092 \quad \mathrm{ps}^{-1}\mathrm{eV}^{-2}, \\
\tilde{c}_1 &= 0.458 \quad \mathrm{ps}^{-1}, \\
\tilde{c}_2 &= 91.138 \quad \mathrm{ps}^{-1}\mathrm{eV}^{-1}, \\
\tilde{c}_3 &= \text{-}87.866 \quad \mathrm{ps}^{-1}\mathrm{eV}^{-2}.
\end{aligned}$$

The relaxation times of viscosity tensor can be taken as constant. The more appropriate value is $\tau_\sigma = 0.02$ ps.

We remark that the above data refer to homogeneous Si material modeled with parabolic bands and with only the electron-phonon scattering (both acoustic and optical) taken into account. In particular, scattering with impurities has been completely neglected.

The generalization of the previous results to the three dimensional situation is straightforward for the production terms of energy and stress, but it presents some difficulties for the momentum and energy flux productions because the generalization of (42, 43) in a tensorial form is not unique.

Two possible generalizations of (42, 43) to the three dimensional case are the following

$$Q_i = -\left(c_1 + c_3 \frac{\mathbf{S} \cdot \mathbf{S}}{\mathbf{J} \cdot \mathbf{S}} \right) F_i + \frac{1}{2} c_2 F_{ill} \tag{44}$$

or

$$Q_i = -c_1 F_i + \frac{1}{2} \left(c_2 + c_3 \frac{\mathbf{S} \cdot \mathbf{J}}{\mathbf{J} \cdot \mathbf{J}} \right) F_{ill}. \tag{45}$$

The same expressions can be introduced for $\tilde{Q}_i$.

In order to choose between (44) and (45), one needs an accurate analysis of two and three dimensional MC simulation in non-homogeneous situations. We will not tackle this question here. It will be considered in a future paper. However we observe that the only component of F_{ill} which is not collinear with F_i is q_i. In turn, q_i can be decomposed into a convective and a diffusive term. If we perform a Maxwellian iteration as in [16], we explicitly get

$$q_i = -\tau_q \frac{n k_B T}{m^*} \frac{\partial T}{\partial x^i} + \frac{5}{2} k_B T \left(\frac{\tau_q}{\tau_q} - 1 \right) F_i$$

where from

$$F_{ill} = v^2 F_i + \frac{5}{2} \frac{\tau_q}{\tau_p} k_B T F_i - \tau_q \frac{n k_B T}{m^*} \frac{\partial T}{\partial x^i}.$$

In practical situation the diffusion term represented by q_i is negligible compared to the convective one and the first term of F_{ill} is small compared to the second one. Therefore the two representations should give the same results within a reasonable degree of approximation.

5 Formal properties

Once the Lagrangian multipliers are known and the expression of the distribution function is set out, in principle it is possible to write explicitly the additional balance law for the entropy of the system [20, 21, 30, 31, 32]. The existence of an additional balance law has important consequences on the mathematical structure of the field equations.

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

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

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 [41]. As a consequence, the initial value problem for this system is well posed [43].

In our case the multipliers have been obtained in an approximate way and the resulting system is not necessarily symmetric hyperbolic. We shall check directly the hyperbolicity of the system in the one dimensional case.

In the one dimensional case the evolution equations read

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(nv) = 0, \tag{46}$$

$$\frac{\partial}{\partial t}(nv) + \frac{\partial}{\partial x}\left(nv^2 + \frac{p}{m^*} + \frac{\sigma}{m^*}\right) = -\frac{nv}{\tau_p} - \frac{neE}{m^*}, \tag{47}$$

$$\frac{\partial}{\partial t}\left(nv^2 + \frac{3p}{m^*}\right) + \frac{\partial}{\partial x}\left(\frac{5vp}{m^*} + \frac{2q}{m^*}\right) = -2\frac{W - W_0}{m^*\tau_W} - \frac{2nevE}{m^*}, \tag{48}$$

$$\begin{aligned} &\frac{\partial}{\partial t}\left(\frac{2}{3}nv^2 + \frac{\sigma}{m^*}\right) + \frac{\partial}{\partial x}\left(\frac{4}{3}\frac{vp}{m^*} + \frac{8}{15}\frac{q}{m^*}\right) = \\ &\qquad -\frac{1}{\tau_\sigma}\left(\frac{2}{3}nv^2 + \frac{\sigma}{m^*}\right) - \frac{4nevE}{3m^*}, \end{aligned} \tag{49}$$

$$\begin{aligned} &\frac{\partial}{\partial t}\left(\frac{5vp}{m^*} + \frac{2q}{m^*}\right) + \frac{\partial}{\partial x}\left[5\frac{p^2}{n(m^*)^2} + 7\frac{\sigma p}{n(m^*)^2} + \frac{32}{5}\frac{qv}{m^*} + 8\frac{pv^2}{m^*} + \frac{148}{25}\frac{q^2}{m^* p}\right] = \\ &\qquad -\frac{1}{\tau_q}\left(\frac{5vp}{m^*} + \frac{2q}{m^*}\right) - \frac{eE}{m^*}\left(3nv^2 + \frac{5p}{m^*} + \frac{2\sigma}{m^*}\right). \end{aligned} \tag{50}$$

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 $\mathbf{U} = (n, v, T, \sigma, q)$, the system is written as

$$A^{(0)}\frac{\partial \mathbf{U}}{\partial t} + A^{(1)}\frac{\partial \mathbf{U}}{\partial x} = \mathbf{f}(\mathbf{U}) \tag{51}$$

We recall that system (51) 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*.

Because of the nonlinearity of the system, this condition may depend on the values of the field $\mathbf{U}$ and can be analyzed in the regions where the solution is regular (where the system can be written in the form (51)).

The first condition on the hyperbolicity is satisfied because for physical values of the solutions $\det A^{(0)} = 6k_B n^2/(m^*)^3 > 0$, while the characteristic equation reads

$$\begin{aligned}
&\lambda\left[\lambda^4 - \left(\frac{8v}{3} + \frac{148q}{25nk_BT}\right)\lambda^3\right.\\
&+\left(\frac{16}{15}v^2 - \frac{26}{5}\frac{k_BT}{m^*} - \frac{17}{15}\frac{\sigma}{nm^*} + \frac{148}{75}\frac{q^2}{(nk_BT)^2} + \frac{148}{15}\frac{vq}{nk_BT}\right)\lambda^2 +\\
&\left(\frac{348}{25}\frac{q}{nm^*} + \frac{8}{5}\frac{\sigma v}{nm^*} - \frac{296}{125}\frac{vq^2}{(nk_BT)^2} - \frac{12}{5}v^3 - \frac{296}{25}\frac{qv^2}{nk_BT} + \frac{48}{5}\frac{vk_BT}{m^*}\right)\lambda\\
&-\frac{7}{5}\frac{\sigma v^2}{nm^*} + \frac{8}{5}v^4 + \frac{148}{25}\frac{qv^3}{nk_BT} - \frac{24}{5}\frac{v^2k_BT}{m^*} + 3\frac{(k_BT)^2}{(m^*)^2} + \frac{21}{5}\frac{k_BT\sigma}{n(m^*)^2}\\
&\left.+\frac{148}{25}\frac{q^2v^2}{(nk_BT)^2} - \frac{348}{25}\frac{vq}{nm^*}\right] = 0. \qquad (52)
\end{aligned}$$

By setting

$$\lambda = \sqrt{\frac{k_BT}{m^*}}\tilde{\lambda}, \quad v = \sqrt{\frac{k_BT}{m^*}}\tilde{v}, \quad q = nm^*\left(\frac{k_BT}{m^*}\right)^{3/2}\tilde{q}, \quad \sigma = nk_BT\tilde{\sigma},$$

the characteristic polynomial becomes

$$\tilde{\lambda}\left[\tilde{\lambda}^4 + \alpha_1\tilde{\lambda}^3 + \alpha_2\tilde{\lambda}^2 + \alpha_3\tilde{\lambda} + \alpha_4\right],$$

with obvious values of the coefficients α_i.

If we introduce the affine transformation

$$\hat{\lambda} = \tilde{\lambda} - \alpha_1/4,$$

the characteristic equation rewrites

$$\hat{\lambda}\left[\hat{\lambda}^4 + \beta_2\hat{\lambda}^2 + \beta_3\hat{\lambda} + \beta_4\right] = 0, \qquad (53)$$

with

$$\begin{aligned}
\beta_2 &= -\frac{26}{5} - \frac{7}{3}\tilde{\sigma} - \frac{88}{75}\tilde{v}^2 - \frac{1628}{375}\tilde{v}\tilde{q} - \frac{20942}{1875}\tilde{q}^2,\\
\beta_3 &= \frac{32}{25}\tilde{v} - \frac{184}{125}\tilde{q} - \frac{14}{15}\tilde{\sigma}\tilde{v} - \frac{518}{75}\tilde{\sigma}\tilde{q} - \frac{1136}{375}\tilde{v}^3 - \frac{6808}{625}\tilde{v}^2\tilde{q} - \frac{113072}{9375}\tilde{v}\tilde{q}^2 - \frac{941872}{46875}\tilde{q}^3,\\
\beta_4 &= 3 + \frac{21}{5}\tilde{\sigma} - \frac{56}{125}\tilde{v}^2 - \frac{556}{625}\tilde{v}\tilde{q} + \frac{28786}{3125}\tilde{q}^2 - \frac{49}{75}\tilde{v}^2\tilde{\sigma} - \frac{518}{375}\tilde{\sigma}\tilde{v}\tilde{q} - \frac{9573}{1875}\tilde{\sigma}\tilde{q}^2\\
&\quad -\frac{11802149}{1171875}\tilde{q}^4 - \frac{651644}{78125}\tilde{q}^3\tilde{v} - \frac{609316}{46875}\tilde{q}^2\tilde{v}^2 - \frac{44548}{9375}\tilde{q}\tilde{v}^3 - \frac{304}{1875}\tilde{v}^4.
\end{aligned}$$

Therefore the hyperbolicity condition depends on the variables $\tilde{v}$, $\tilde{\sigma}$ and $\tilde{q}$ (of course the affine transformation $\tilde{\lambda} \mapsto \tilde{\lambda} - \alpha_1/4$ does not change the hyperbolicity region in the $(\tilde{v}, \tilde{q}, \tilde{\sigma})$-space).

Firstly we show that the hyperbolicity region is not empty. For $\tilde{v} = \tilde{q} = \tilde{\sigma} = 0$ it is immediate to see that the system is strictly hyperbolic and the eigenvalues are given by

$$\begin{aligned} \hat{\lambda} &= 0, \\ \hat{\lambda} &= \pm\sqrt{\frac{1}{5}(13 \pm \sqrt{94})}. \end{aligned}$$

We expect the system to be hyperbolic in a neighborhood of the origin in the $(\tilde{v}, \tilde{\sigma}, \tilde{q})$-space.

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

$$\hat{\lambda}(\hat{\lambda} - \hat{\lambda}_1)^2(\hat{\lambda} - \hat{\lambda}_2)(\hat{\lambda} - \hat{\lambda}_3) = 0. \tag{54}$$

By comparing (53) with (54), one has

$$\hat{\lambda}_1 + \frac{1}{2}(\hat{\lambda}_2 + \hat{\lambda}_3) = 0, \tag{55}$$

$$\hat{\lambda}_1^2 + 2\hat{\lambda}_1(\hat{\lambda}_2 + \hat{\lambda}_3) + \hat{\lambda}_2\hat{\lambda}_3 = \beta_2, \tag{56}$$

$$\hat{\lambda}_1^2(\hat{\lambda}_2 + \hat{\lambda}_3) + 2\hat{\lambda}_1\hat{\lambda}_2\hat{\lambda}_3 = \beta_3, \tag{57}$$

$$\hat{\lambda}_1^2\hat{\lambda}_2\hat{\lambda}_3 = \beta_4. \tag{58}$$

By solving the previous system, one obtains that the hyperbolicity region is the connected component, containing the origin, of the set whose boundary is given by the curves of equations

$$\beta_3 = \pm\eta\left(\frac{\eta^2}{2} + \beta 2\right), \tag{59}$$

where

$$\eta = \sqrt{\frac{2}{3}\left(-\beta_2 \pm \sqrt{\beta_2^2 + 14\beta_4}\right)}.$$

Fig. 1 shows the hyperbolicity region in the ($\tilde{\sigma}$ - $\tilde{q}$) plane for several values of $\tilde{v}$. When $\tilde{v} \approx 0$ there are practically not limits on $\tilde{\sigma}$ and $\tilde{q}$. If the value of $\tilde{v}$ is increased, bounds on the normalized heat flux appear. These limitations are relevant only for $|\tilde{v}|$ greater than 0.7. However in the simulation of real electron devices such values of $\tilde{v}$ are not usually met and therefore we expect that our model satisfies the hyperbolicity condition in the cases of practical applications.

6 Numerical method

Numerical integration of quasi-linear hyperbolic systems represents by itself an active research area (see [44]). It is well known that the solutions of quasi-linear systems suffer loss of regularity and formation of shocks. In the last decade accurate shock capturing schemes have been developed, such as ENO schemes [45]. However, high order upwind-based shock capturing schemes require the explicit knowledge of the characteristic speeds of the hyperbolic system. In the case of the model presented in the previous section, it is not possible to obtain analytical expressions for the eigenvalues and eigenvectors of the system, and it is therefore not practical to use upwind-based ENO schemes in order to integrate Eqs. (46)-(50). The scheme proposed by Nessyahu and Tadmor (NT) [26] uses Lax-Friedrichs scheme as building block, corrected by MUSCL-type interpolation so that it becomes second order accurate in smooth regions. It does not require the knowledge of the characteristic structure and it is therefore particularly suited for the system (46)-(50). NT scheme has been developed for homogeneous systems. Here we use a suitable extension of the method to systems that contain production terms.

The complete method is based on a splitting technique. The NT scheme is used for the convection step, while the relaxation step is solved by some unconditionally stable scheme [25]. Here we shall briefly recall the method.

Let us consider a system of the form

$$\frac{\partial v}{\partial t} + \frac{\partial F(v)}{\partial x} = G(v), \tag{60}$$

with $v \in \mathbf{R}^m$ and $F : \mathbf{R}^m \to \mathbf{R}^m$.

The basic idea is to integrate first the relaxation system (relaxation step),

$$\frac{dv}{dt} = G(v). \tag{61}$$

and then the homogeneous system (convection step), using the output of the previous step as initial condition.

$$\frac{\partial v}{\partial t} + \frac{\partial F(v)}{\partial x} = 0, \tag{62}$$

We use NT scheme with a staggered grid for the convection step.

Each step has the form of predictor-corrector scheme:

$$v_{j+1/2}^{n+1/2} = \frac{1}{2}(v_j^{n+1} + v_{j+1}^n) + \frac{1}{8}(v_j' - v_{j+1}') - \lambda\left[F(v_{j+1}^{n+1/2}) - F(v_j^{n+1/2})\right], \tag{63}$$

$$v_j^{n+1/2} = v_j^n - \frac{\lambda}{2}F_j'. \tag{64}$$

where $\lambda = \Delta t/\Delta x$. The time step Δt must satisfy a stability condition

$$\lambda \cdot \max \rho(A(v(x,t)) < \frac{1}{2} \tag{65}$$

where $\rho(A(v(x,t))$ is the spectral radius of the Jacobian matrix,

$$A = \frac{\partial F}{\partial v}.$$

This condition will ensure that the generalized Riemann problems with piece-wise smooth data at time t_n will not interfere during the time step Δt.

In order to couple the convection step with the relaxation step, it is convenient to make two convection steps of step size $\Delta t/2$, so that the solution is computed on the same grid. A complete convection step of step size Δt is obtained as a sequence of two intermediate steps of step size $\Delta t/2$.

The values of $v'_j/\Delta x$ and $F'_j/\Delta x$ are a first order approximation of the space derivatives of the field and of the flux, computed from cell averages by using Uniform Non Oscillatory reconstruction (UNO, see [45]),

$$v'_j = \mathrm{MM}\left(d_{j-\frac{1}{2}}v + \frac{1}{2}\mathrm{MM}(D_{j-1}, D_j), d_{j+\frac{1}{2}}v - \frac{1}{2}\mathrm{MM}(D_j, D_{j+1})\right) \tag{66}$$

where

$$D_j = v_{j+1} - 2v_j + v_{j-1},$$

$$d_{j+1/2} = v_{j+1} - v_j.$$

and

$$\mathrm{MM}(x,y) = \begin{cases} \mathrm{sign}(x)\cdot\min(|x|,|y|) & \text{if } \mathrm{sign}(x) = \mathrm{sign}(y) \\ 0 & \text{otherwise.} \end{cases}$$

A similar procedure is used for computing F'_j.

For the relaxation step an unconditionally stable second order scheme can be obtained by analytical integration of the linearized relaxation equation, where linearization is obtained by *freezing* the coefficients at time t_n. The electric potential is computed by solving with standard procedure the tridiagonal system

$$\epsilon(\phi_{j+1} - 2\phi_j + \phi_{j-1}) = -e(\Delta x)^2\left(N_D - N_A - n_i^n\right)$$

and the electric field has been obtained by the electric potential using finite differences.

Eq. (61) can be written explicitly as

$$\begin{aligned}
\frac{dn}{dt} &= 0, \\
\frac{dJ}{dt} &= -\frac{J}{\tau_p} - \frac{neE}{m^*}, \\
\frac{dW}{dt} &= \frac{W - 3nk_BT_0/2}{\tau_W} - JeE, \\
\frac{dV}{dt} &= -\frac{V}{\tau_\sigma} - \frac{4JeE}{3m^*}, \\
\frac{dS}{dt} &= -\frac{S}{\tau_q} - \frac{eE}{2m^*}\left(3nv^2 + \frac{5p}{m^*} + \frac{2\sigma}{m^*}\right),
\end{aligned}$$

with $V = F_{<11>}$.

By evaluating the relaxation times and the electric field at $t = t_n$, we can integrate numerically the equations for density, energy and shear as

$$
\begin{aligned}
n_j^{n+1} &= n_j^n, \\
J_j^{n+1} &= J_j^n \exp\left(\frac{\Delta t}{\tau_{pj}^n}\right) - d_1\left(1 - \exp\left(\frac{\Delta t}{\tau_{pj}^n}\right)\right) \\
W_j^{n+1} &= \frac{3n_j^n k_B T_0}{2} + \left(W_j^n - \frac{3n_j^n k_B T_0}{2}\right)\exp\left(-\frac{\Delta t}{\tau_{W_j}^n}\right) - d_2\left(1 - \exp\left(-\frac{\Delta t}{\tau_{W_j}^n}\right)\right), \\
V_j^{n+1} &= V_j^n \exp\left(\frac{\Delta t}{\tau_{\sigma_j}^n}\right) - d_3\left(1 - \exp\left(-\frac{\Delta t}{\tau_{\sigma_j}^n}\right)\right), \\
S_j^{n+1} &= S_j^n \exp\left(\frac{\Delta t}{\tau_{qj}^n}\right) - d_4\left(1 - \exp\left(\frac{\Delta t}{\tau_{qj}^n}\right)\right).
\end{aligned}
$$

The coefficients d_i are given by

$$
\begin{aligned}
d_1 &= \frac{n_j^n e E_j^n}{m^*}, \\
d_2 &= J_j^n e E_j^n \tau_W, \\
d_3 &= \frac{4 J_j^n e E_j^n \tau_{\sigma_j}^n}{3m^*}, \\
d_4 &= \frac{e E_j^n}{2m^*}\left(3 J_j^n v_j^n + \frac{5 p_j^n}{m^*} + \frac{2\sigma_j^n}{m^*}\right).
\end{aligned}
$$

The time step is chosen in order to satisfy condition (65) on the eigenvalues of the matrix A.

The splitting technique that we just presented is first order in time. It is possible to obtain second order accuracy in time by combining the two steps according to the following scheme [24, 25]. Given the field at time t_n, (U^n, E^n), the field at time $t_{n+1/2}$ is obtained by

$$
\begin{aligned}
U_1 &= U^n - R(U_1, E^n, \Delta t), \\
U_2 &= \frac{3}{2}U^n - \frac{1}{2}U_1, \\
U_3 &= U_2 - R(U_3, E^n, \Delta t), \\
U_4 &= \mathcal{C}_{\Delta t} U_3, \\
E^{n+1} &= \mathcal{P}(U_4), \\
U^{n+1} &= U_4 - R(U^{n+1}, E^{n+1}, \Delta t/2)
\end{aligned}
$$

where R represents the discrete operator corresponding to the relaxation step, $\mathcal{C}_{\Delta t}$ is the discrete operator corresponding to NT scheme, and $\mathcal{P}(U)$ gives the solution to Poisson's equation.

7 Numerical results

As test problem we consider a ballistic diode $n^+ - n - n^+$, which models a MOSFET channel. The diode is made of silicon, and the bulk temperature is supposed to be 300°K. The n^+ regions are $0.1\mu m$ long.

Three test cases have been considered, which differ in the channel length and in the doping profile. The parameters are shown in the following table.

Test #	Channel length L_c (μm)	N_D^+ ($\times 10^{17}$ cm^{-3})	N_D ($\times 10^{17}$ cm^{-3})
1	0.4	5	0.02
2	0.3	10	0.1
3	0.2	10	0.1

For the electron effective mass in the approximation of parabolic band we use $m^* = 0.32\ m_e$ when m_e is the electron mass [46]. Silicon dielectric constant is given by $\epsilon = \epsilon_r \epsilon_0$, where ϵ_r =11.7 is the relative dielectric constant and $\epsilon_0 = 8.85 \times 10^{-18} C/V\mu m$ is the dielectric constant of vacuum.

The initial electron temperature is the lattice temperature $T_0 = 300°$K and the charges are at rest. A bias voltage of 1 Volt is applied, and this determines a charge flux in the semiconductor.

The initial conditions for the system are

$$n(x,0) = n_0(x),\ T(x,0) = 300°\mathrm{K},\ v(x,0) = 0,\ q(x,0) = 0,\ \sigma(x,0) = 0. \quad (67)$$

The doping profile is regularized according to the function

$$n_0(x) = n_0 - d_0 \left(\tanh \frac{x - x_1}{s} - \tanh \frac{x - x_2}{s} \right),$$

where $s = 0.01\mu$m, $n_0 = n_0(0)$, $d_0 = n_0(1 - N_D/N_D^+)/2$, $x_1 = 0.1\mu$m, and $x_2 = x_1 + L_c$ with L_c channel length. The total length of the device is $L = L_c + 0.2\mu$m.

Regarding the boundary conditions, in principle the number of independent conditions on each boundary should be equal to the number of characteristics entering the domain. However, in the highly doped regions, one is close to thermodynamic equilibrium, therefore in that part of the device the nonlinear effects are negligible and the results should be very close to those obtained for model obtained by Maxwellian iteration [22]. Numerical results show that in the latter the solution is flat near the boundary. This justifies the use of the following boundary conditions

$$\begin{aligned}
n(0,t) &= n(L,t) = N_D^+ && (68)\\
\frac{\partial}{\partial x} v(0,t) &= \frac{\partial}{\partial x} v(L,t) = 0, && (69)\\
\frac{\partial}{\partial x} T(0,t) &= \frac{\partial}{\partial x} T(L,t) = 0, && (70)\\
e\phi(0) &= T_0 \ln\left(\frac{n(0)}{n_i}\right), \qquad e\phi(L) = T_0 \ln\left(\frac{n(L)}{n_i}\right) + eV_b, && (71)
\end{aligned}$$

where $n_i = 1.4 \times 10^{10}$ cm^{-3} is electron intrinsic concentration, and V_b is the applied bias voltage.

From the continuity equation, and from conditions (68, 69, 70) it follows

$$\begin{aligned}
\frac{\partial J}{\partial x}(0,t) &= \frac{\partial J}{\partial x}(L,t) = 0 \\
\frac{\partial W}{\partial x}(0,t) &= \frac{\partial W}{\partial x}(L,t) = 0 \\
\frac{\partial S}{\partial x}(0,t) &= \frac{\partial S}{\partial x}(L,t) = 0
\end{aligned}$$

There is no sign of spurious oscillations near the boundary, indicating that the boundary conditions are in fact compatible with the solution of the problem.

We observed that during the transient the solutions may leave the hyperbolicity region due to oscillations near the junctions. To overcome this problem we have adopted initially a very restrictive CFL condition. Then, once a solution close to the stationary one has been obtained, we continued the computation by using $\Delta t = \Delta x/2c_s$ for the test problem 1, $\Delta t = \Delta x/2.5c_s$ for the test problem 2, $\Delta t = \Delta x/3c_s$ for the test problem 3, c_s being $\sqrt{k_B T_0/m^*}$.

The stationary solution is reached within a few picoseconds (about five). For the test case 2 we have performed the simulations with 120 and 240 grid points. As shown in Fig. 2 there are noticeable differences only near the junctions, where the electric field has the greatest intensity. Therefore for the applications it is sufficient to consider only 120 grid points.

In all cases we have treated we notice the presence of an irregular behavior located almost at the end of the second junction. This anomalous effect is more pronounced for the momentum (see Fig. 2(d)); indeed the latter is not conserved in the stationary regime, but presents a deviation from constancy near the first junction and a sharp spike near the second junction. A refinement of the spatial mesh shows that the first irregularity is of numerical type and it is negligible with 240 grid points. Concerning the second effect, the spike is enhanced by smaller mesh size, which is an indication of the occurrence of some sort of "singularity" in the stationary solution. By computing the Jacobian throughout the stationary solution one finds that the location of the singularity corresponds to a point where the Jacobian vanishes but where the compatibility with the RHS is not satisfied. The irregularity seems to be more singular than a shock and suggests the presence of a delta-shock (see [48] and references therein). An assessment of the various possibilities requires a much more detailed analysis. We remark that in the case of extended thermodynamics of a mono atomic rarefied gas with Maxwell molecules, the numerical simulations of [42] show that no singularity occurs at the points where the Jacobian vanishes (in the stationary solution) because the compatibility condition is automatically satisfied. To the authors knowledge no satisfactory mathematical explanation of this phenomenon has been found yet. A possible approach could be the extension of viscosity solution methods to the system under consideration. Such techniques have been used in [49] in the case of a simpler problem consisting of two balance equations.

It is remarkable that our numerical scheme is capable of providing a sensible solution which is regular everywhere except at some singular point and which agrees reasonably well with the MC simulations. This perhaps could be ascribed to the fact that our scheme solves the non stationary equations and the stationary solution is approached with a limiting process.

The numerical results found for the stationary case with 120 grid points have been compared with the Monte Carlo results obtained by the DAMOCLES code [2].

Numerical solutions show for the test case 1 and 2 a good agreement with a discrepancy at most of about 10% (see Fig. 2 and Fig. 3) for all the fields except the heat flux (Fig. 2c and Fig. 3c). We observe that the relaxation times given in [15] are obtained without considering the scattering with crystal impurities. Therefore the effective relaxation times could be shorter due to the additional scattering mechanism. This could be a partial explanation of the discrepancy. A meaningful comparison with MC simulations would require that the relaxation times (Eqs.24-25) be fitted to the results of homogeneous MC simulations but at various levels of impurities concentrations and taking into account scattering with impurities.

Test case 3 shows a good agreement for the energy and the heat flux is described better than the previous case, but the results of the velocity are not satisfactory. Probably in such a limiting case (which presents a situation very far from thermodynamical equilibrium and a regime where the fluid approach is suspicious and a full kinetic description could be mandatory) a more accurate description must be followed by increasing the number of the moments and improving the accuracy of the closure relations.

Finally we remark that the effect of viscosity is negligible and in the applications it is sufficient to consider only the inviscid case.

Conclusions

A new hydrodynamical model has been presented for charge transport in semiconductors. The model is based on Extended Thermodynamics, and constitutes an improvement of a previous model presented in [16, 15]. A robust and accurate numerical method has been developed, which is suitable for the mathematical structure of the model, and a comparison has been performed with detailed Monte Carlo simulations.

The results of the comparison are quite satisfactory, since the agreement with Monte Carlo is observed in all the field variables with a discrepancy of about 10%, at least for the cases considered here.

One of the main open problems is the determination of the coefficients of the production terms. The entropy principle does not allow to determine them. They have been considered as phenomenological functions, expressed by fitting MC data in the homogeneous case. We want to stress that the expression given for the relaxation times do not depend on the particular simulated device, but only on the homogeneous material, because of the local dependence on the macroscopic variables.

We want to remark that our hydrodynamical model can also be successfully used for perturbation analysis of a given device under given operating conditions. In a perturbation approach the basic transport parameters appearing in the closure and production terms will be those of the unperturbed state. By linearizing the equations around the unperturbed state one obtains an analytical linear boundary value problem which leads itself to analytical linear analysis.

At this point the same numerical technique used to solve the unperturbed problem can be used to solve the perturbed problem in order to obtain important physical quantities, e.g. the impedance matrix in the small signal analysis (see [50] for the $n^+ - n - n^+$ InP diode).

We used a versatile numerical technique, easily implementable in computer codes. It makes it easy to change closures and models for the production terms. It automatically solves also the non-stationary problem. The authors are presently working to a 2D extension of the numerical scheme, in order to treat devices with a more complex geometry.

The universality of our models remains to be checked by considering different channel lengths, applied voltages and doping profiles. This require an extensive database of MC simulations which is under current construction.

Acknowledgments

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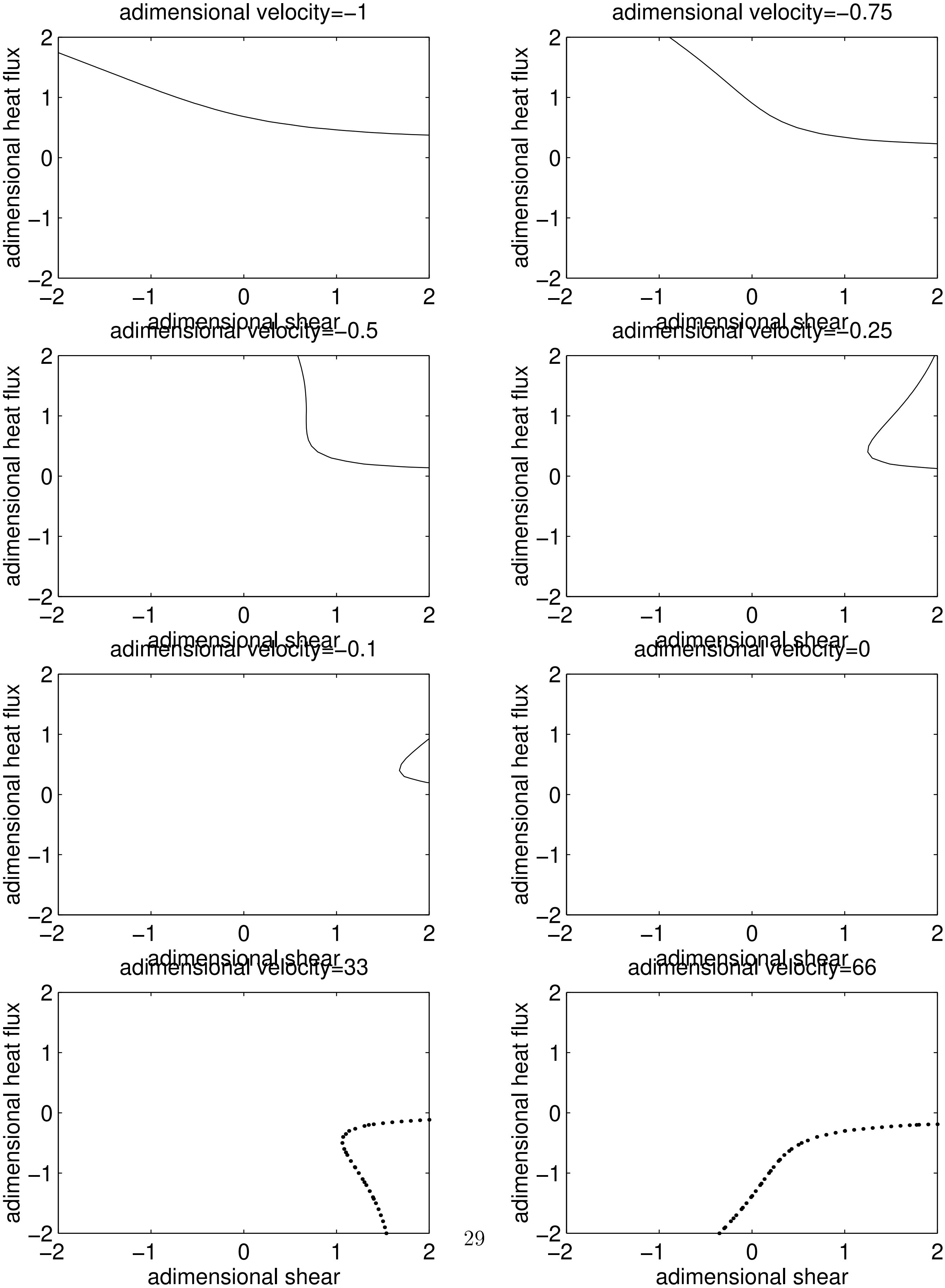

Figure 1: Hyperbolicity region for several values of $\tilde{v}$. For low values of $\tilde{v}$ the range of variability of $\tilde{q}$ and $\tilde{\sigma}$ is practically not limited. By increasing the absolute value of $\tilde{v}$ some bounds arise for $\tilde{q}$ and $\tilde{\sigma}$, but they allow to satisfy the hyperbolicity condition in the concrete cases arising in the applications.

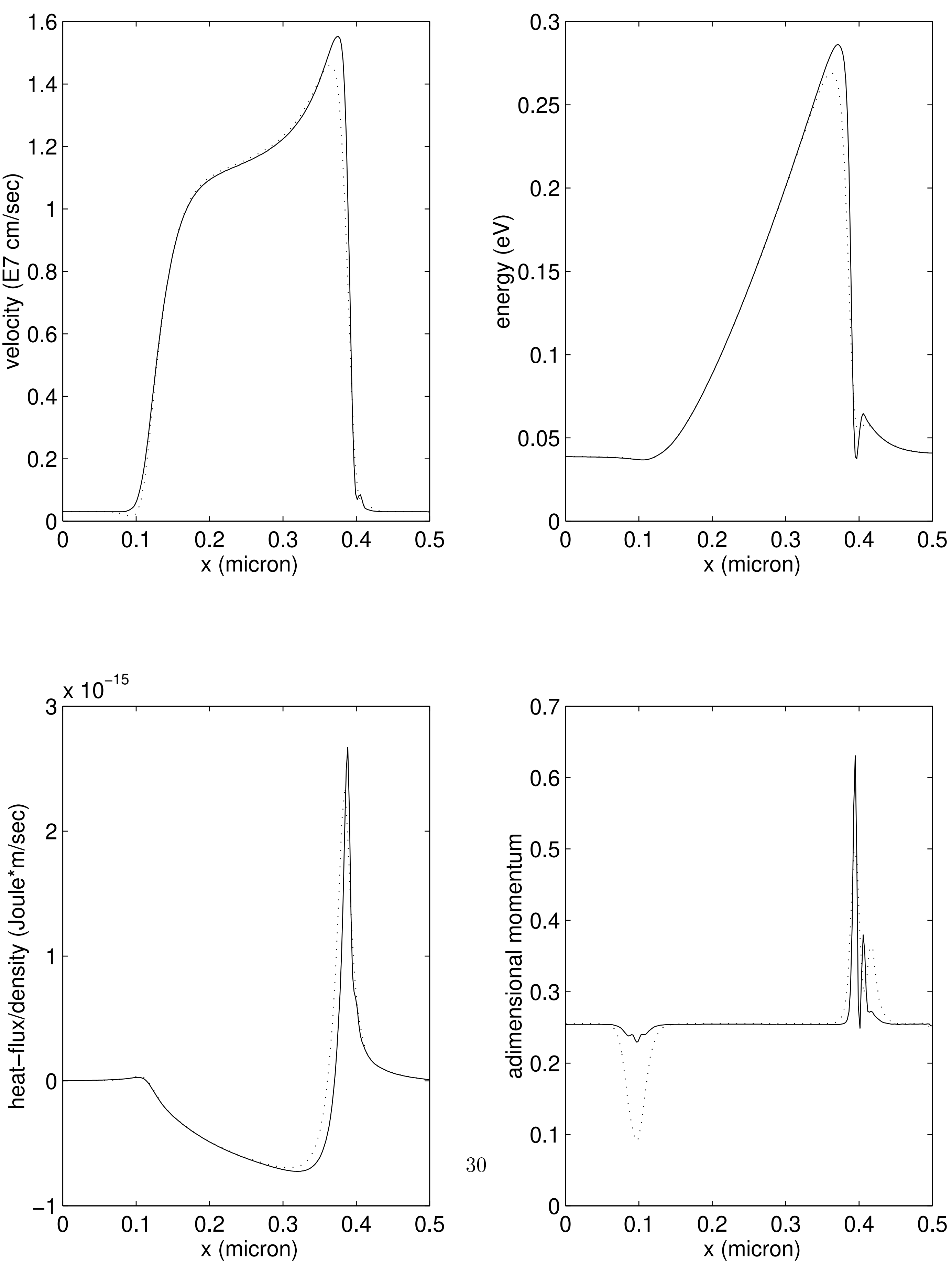

Figure 2: **Fig. 2**. Comparison between the stationary solution obtained for the case of channel of length 0.3 μm with 120 (dashed line) and 240 grid points (continuous line) for the following fields: velocity (a), energy (b), heat flux (c), momentum (d).

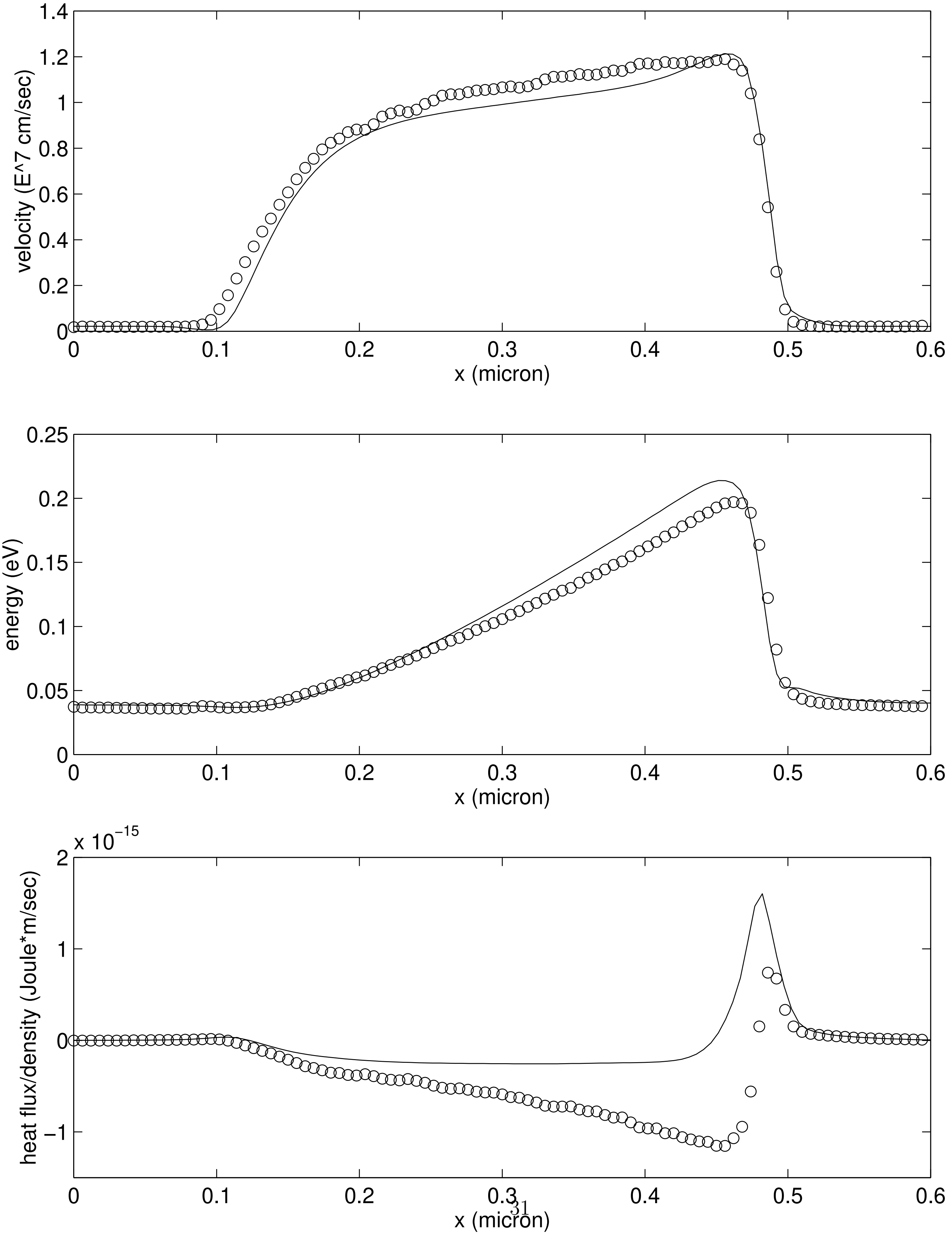

Figure 3: Numerical results for the test case 1 (continuous line) obtained with 120 grid points compared with the MC results (circles).

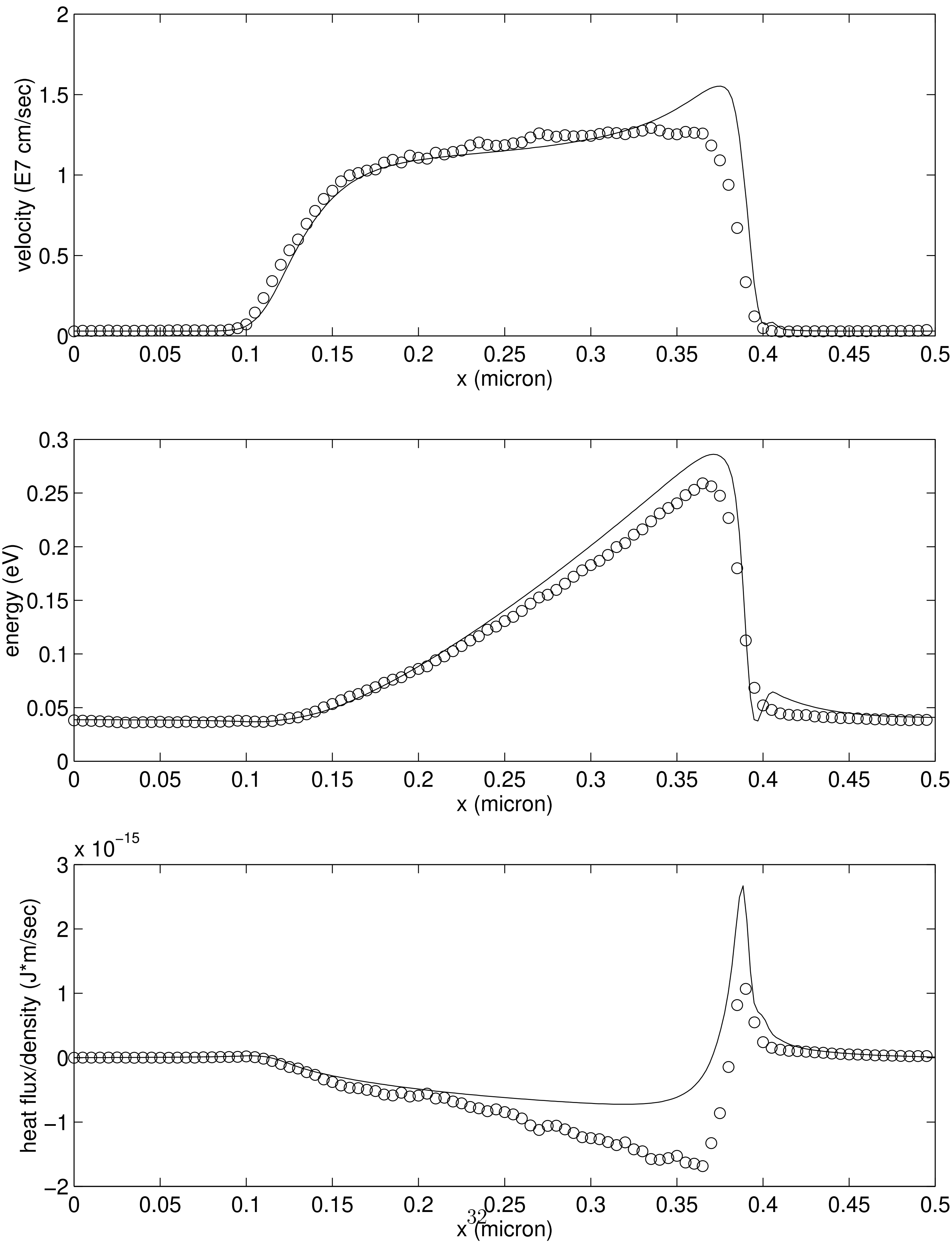

Figure 4: Numerical results for the test case 2 (continuous line) obtained with 120 grid points compared with the MC results (circles).

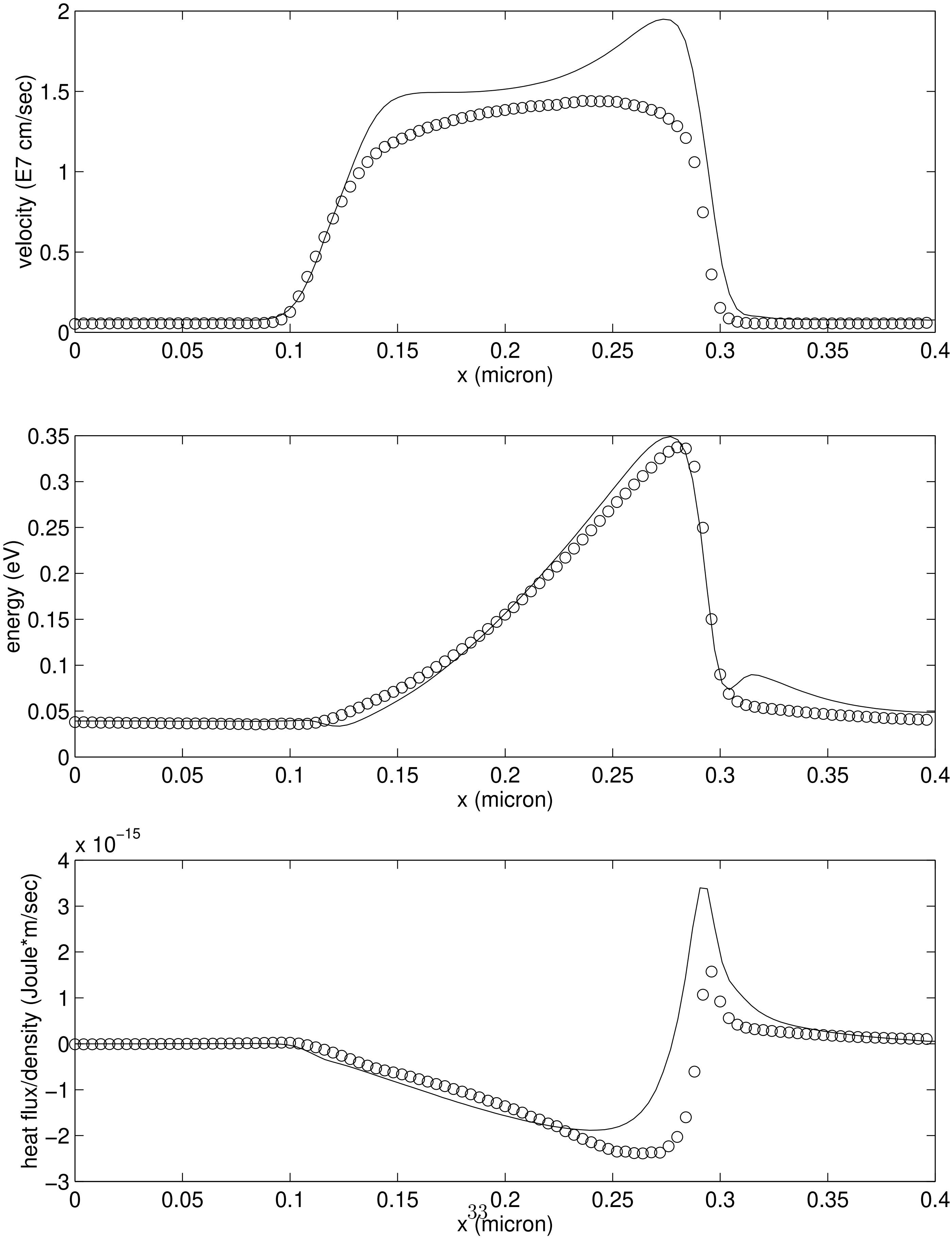

Figure 5: Numerical results for the test case 3 (continuous line) obtained with 120 grid points compared with the MC results (circles).