TRANSPORT EFFECT, HYPERBOLICITY, AND SHOCK CAPTURING ALGORITHMS FOR DEVICE SIMULATIONS

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Abstract

We study the effect of the common practice of neglecting the convective terms (inertial approximation) in the hydrodynamic model in the simulation of n^+-n-n^+ diodes and two dimensional MESFET devices. We find that the inertial approximation is invalid near the diode junctions, and near the contact regions of the MESFET device. We also test the hyperbolicity of the first derivative part in the hydrodynamic model, and in related energy transport models. We find that the first derivative part of the system is hyperbolic, for the hydrodynamic model, the modified hydrodynamic model, and the energy transport model. This suggests and validates the use of shock capturing algorithms for the simulation.

I. TRANSPORT EFFECT.

In earlier work (see [5]), we have advocated using modern nonlinear hyperbolic based shock capturing algorithms (e.g., the ENO algorithm in [11]) in device simulations with hydrodynamic (HD) and energy transport (ET) models. Introductions to these models may be found in [10] and [7], respectively. The first use of such methods in device simulation was [2].

A common practice in the interpretation of the hydrodynamic model is to employ the inertial approximation, which in our terminology characterizes the transport effect as small if

$$\tau_p \sqrt{u_x^2 + u_y^2 + v_x^2 + v_y^2} << 1, \tag{1}$$

where τ_p is the momentum relaxation coefficient and (u, v) is the velocity vector. The reader can find this approximation employed in many reduced hydrodynamic models (cf. [9]). As discussed in [10], it allows the extension of the Scharfetter-Gummel method to a hydrodynamic model setting. This hypothesis is well known in fluid mechanics, where the resulting flow is termed a Stokes' flow. In the electrical engineering community, one speaks of neglecting the convective terms.

In this work, we simulate the standard one dimensional n^+-n-n^+ channel and a two dimensional MESFET, using the complete HD model, as introduced in [10], with Baccarani-Wordeman relaxation expressions (see [1]), and then check the validity of (1). From a physical point of view, we wish to check whether the transport effect is uniformly small. If it is, hyperbolic based algorithms probably need not be used, and the inertial approximation would appear justified. The numerical scheme we use is the ENO (Essentially Non-Oscillatory) scheme [11], adapted to device simulations in [2] and [5]. It has the advantage of both high order accuracy and monotone sharp gradient transitions.

The one dimensional n^+-n-n^+ channel is a standard silicon diode with a length of $0.6\mu m$, with a doping defined by $n_d = 5\times 10^5 \mu m^{-3}$ in $[0, 0.1]$ and in $[0.5, 0.6]$, and $n_d = 2\times 10^3 \mu m^{-3}$ in $[0.15, 0.45]$,

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joined by smooth junctions. The lattice temperature is taken as $T_0 = 300$ K. We apply a voltage bias of $vbias = 0.5$V, 1.0V and 1.5V, respectively. Other relevant parameters can be found in [5]. We use a high order ENO scheme (third order) and a very refined grid (200 points), in order to ensure that the physical model is fully resolved by our numerical result.

Fig. 1 (left) clearly shows that the transport effect (the quantity in Eqn. (1)) is *not* small near the junctions. In order to verify that this is not an artifact of the spurious velocity overshoot at the right junction, we also simulate with a reduced heat conduction coefficient $\kappa_0 = 0.5$ to reduce this spurious overshoot (see [4]). The result, Fig. 1 (right), still shows significant transport effect at the junctions, especially at the left junction.

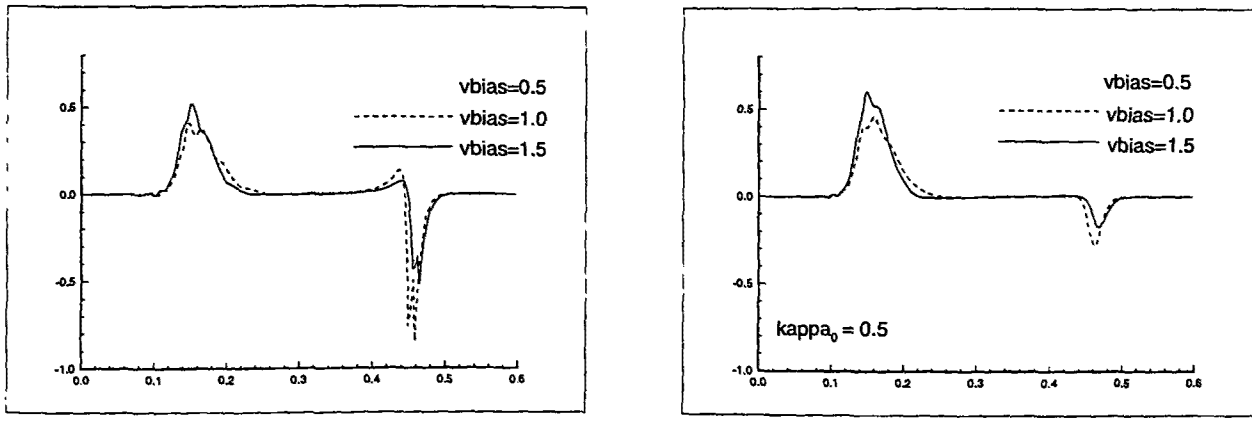


Fig. 1: The transport effect $\tau_p u_x$ for the one dimensional n^+-n-n^+ channel. Left: the HD model; right: the HD model with a reduced heat conduction coefficient $\kappa_0 = 0.5$.

To see the effect of ignoring this transport effect and using a reduced hydrodynamic model, we also make the simulation of the same diode using the reduced HD model with the inertial assumption. This reduced HD model does not have a momentum equation, is a fully parabolic system, hence is much easier to solve numerically. The velocity is a derived quantity from the concentration and energy. We can see from Fig. 2 that the reduced HD model underestimates the velocity.

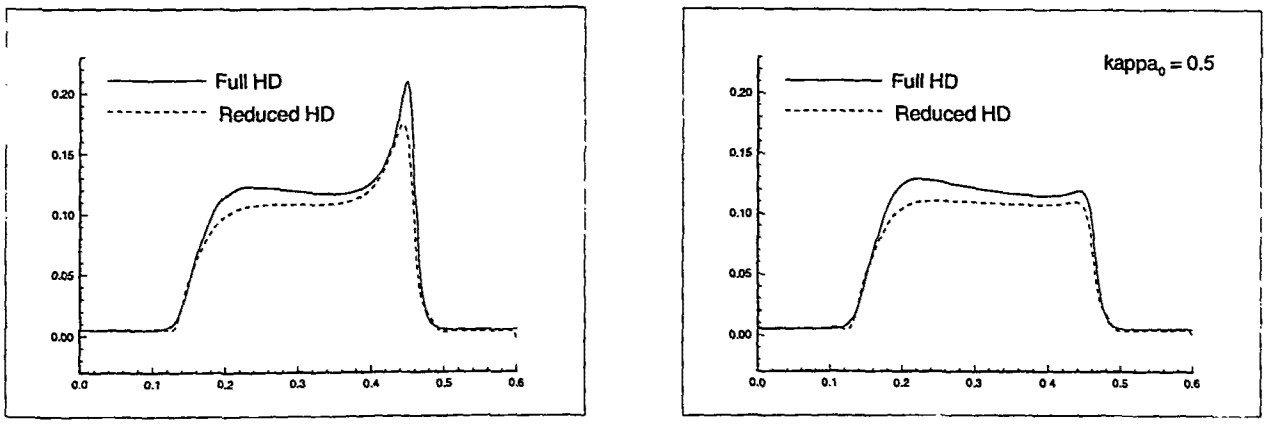
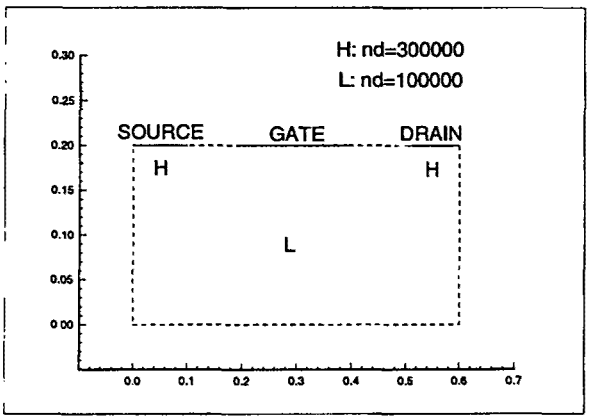


Fig. 2: Velocity at $vbias = 1.5$. Left: the HD model and the reduced HD model; right: the same with a reduced heat conduction coefficient $\kappa_0 = 0.5$.

Next we simulate a two dimensional MESFET of the size $0.6 \times 0.2\mu m^2$. The geometry as well as the doping (in μm^{-3}) is shown in Fig. 3, left. We apply, at the drain, a voltage bias

$vbias = 2$V. The gate is a Schottky contact, with a negative voltage bias $vgate = -0.8$V and a very low concentration value $n = 3.8503 \times 10^{-8} \mu m^{-3}$. The lattice temperature is again taken as $T_0 = 300$ K. A high order (third order) ENO scheme with a very refined grid of 192×64 points is used. Again, this is to ensure that the physical model is fully resolved by the numerical scheme. Boundary conditions and other parameters can be found in [5].

Fig. 3, right, shows that the transport effect is *not* small near the contacts. For easy presentation, we have listed an integer at every other grid point in the MESFET in Fig. 3, right. This integer is ten times the transport effect formula in Eqn. (1), capped from above by nine.



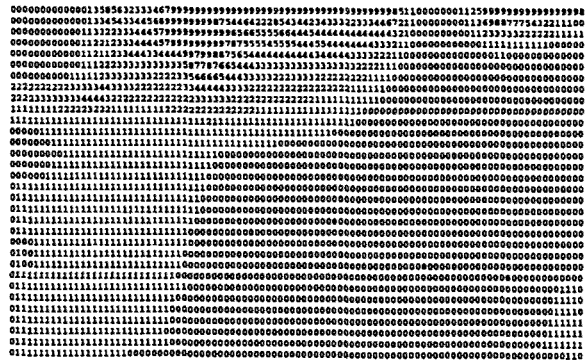


Fig. 3: Two dimensional MESFET. Left: the geometry and the doping n_d; Right: the transport effect. The integers denote the integer part of ten times the transport effect: $\left[10\tau_p \sqrt{u_x^2 + u_y^2 + v_x^2 + v_y^2} \right]$. If it is larger than 9, then 9 is shown.

From these two examples we can conclude that, in device simulations, the transport effect is not uniformly small. This justifies the usage of hyperbolic based shock capturing schemes (e.g., [5]) for device simulation. It also justifies the usage of the full HD model.

II. TEST FOR HYPERBOLICITY.

In this section, we would like to discuss the hyperbolicity check of the first derivative part in the following Eqn. (2), for the HD model, the modified HD model in [13], and for the ET model in [7]. Both HD and ET models can be expressed in the following form:

$$w_t + f_1(w)_x + f_2(w)_y = r(w), \tag{2}$$

where the right-hand-side $r(w)$ contains both the forcing terms due to the relaxation, which are nonlinear functions of w, and the second derivative terms due to the heat conduction. The analysis of the first derivative component of the HD and ET models should not be confused with the mathematical classification of the complete systems (2). Exclusive of the Poisson equation, these are classified as parabolic/hyperbolic and parabolic, respectively. Such classification can be found in, e.g., [3]. Since we are interested in the situation that higher derivatives in the system have relatively small coefficients, and first derivative terms are either dominant or at least are significant, we will study only the first derivative part.

The definition of the first derivative part $f_1(w)_x + f_2(w)_y$ as hyperbolic is: $\xi_1 f_1'(w) + \xi_2 f_2'(w)$ with real ξ_1 and ξ_2, has only real eigenvalues and a complete set of eigenvectors. If the first derivative part is hyperbolic, and if the first derivative part dominates the system or is at least significant, then hyperbolic based algorithms (like ENO) can be very effective. On the other hand,

if the first derivative part is not hyperbolic, the system is of mixed hyperbolic-elliptic type, and the mathematical theory about the solution to (2), when the right-hand-side tends to zero, is very complicated and in many cases still unsolved. Likewise, numerical methods for such mixed type systems are also complicated and under developed (see e.g., [12]). We would thus desire to avoid the appearance of mixed type first derivative part when modifying the models. Notice also that in many modifications to the hydrodynamic models (e.g., [13],[8]), the right-hand-side of Eqn. (2) is changed to contain some first derivative terms also. Although in practical computations these terms are treated as small perturbations and approximated separately, the justification that these terms are indeed "small" can only come from moving these terms to the left-hand-side, absorbing them into $f_1(w)$ and $f_2(w)$, and then checking hyperbolicity. We have performed such a hyperbolicity check for the standard HD model, the modified HD model [13], and the ET model [7]. It is found that all three cases have hyperbolic first derivative parts. The details can be found in [6]. We have to resort to numerical techniques to check the hyperbolicity of the first derivative part for the modified HD model in [13].

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