# A Non-Parabolic Six Moments Model for the Simulation of Sub-100 nm Devices

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Macroscopic transport models based on the first six moments of Boltzmann's equation [1] are a natural extension to the well known drift-diffusion (DD) model (two moments) and the various hydrodynamic and energy-transport models (three or four moments) [2]. In addition to the solution variables of the energy-transport (ET) model, which are the carrier concentration $n = \langle 1 \rangle$ and the average energy $w_1 = \langle \mathcal{E} \rangle$, the six moments (SM) model provides $w_2 = \langle \mathcal{E}^2 \rangle$. The quantity $\beta = (3/5) w_2 / w_1^2$ is the kurtosis of the distribution function and indicates the deviation from a heated Maxwellian distribution for which $\beta = 1$ holds (for parabolic bands). Here we present results of numerical solutions of consistent DD, ET, and SM models and compare them to self-consistent analytic-band [3] and full-band [4] Monte Carlo (MC) simulation results.

The non-parabolic stationary balance and flux equations of the macroscopic moment models are given in [5]. The mobilities, the relaxation times, and the non-parabolicity factors where taken from tabulated bulk data of respective MC simulations and modeled as a function of the average energy only. A critical issue is the modeling of the closure relation for the highest-order moment which was required to be consistent with bulk MC simulations. In addition to the SM model we consider the corresponding ET model, where the equation for $w_2$ is kept but the equation for the energy-flux $\mathbf{V}_1$ is closed with $w_2 = (5/3) w_1^2$, corresponding to a heated Maxwellian distribution. The equation for $w_2$ is therefore decoupled from the lower order equations and provides an estimate for $w_2$ and thus $\beta$ [1, 6].

To investigate the accuracy of the SM model and its corresponding ET model we consider a series of one-dimensional $n^+$-$n$-$n^+$ structures simulated with a maximum electric field of $300\,\mathrm{kV/cm}$. A comparison of the average velocity $\mathbf{V}_0$ and the kurtosis $\beta$ obtained from the macroscopic models with the analytic-band MC simulation is shown in Fig. 1 for three devices. The spurious velocity overshoot is significantly reduced in the SM model, consistent with previous results [7], while the kurtosis produced by the decoupled SM (ET) model is only a poor approximation to the MC results for shorter channel lengths. An accurate kurtosis, however, is a prerequisite for modeling hot carrier effects. The terminal currents as a function of the channel length are shown in Fig. 2, where the ET model shows the well known overestimation for $L_\mathrm{c} \leq 100\,\mathrm{nm}$ while the DD model underestimates for $L_\mathrm{c} \leq 500\,\mathrm{nm}$. The SM model stays close to the MC results down to $L_\mathrm{c} = 40\,\mathrm{nm}$.

In addition we simulated the $50\,\mathrm{nm}$ double-gate MOSFET from [8] and compared the results to self-consistent full-band MC results. To avoid empirical surface scattering models, where consistency between all models is difficult to obtain, we omit surface scattering altogether for the present comparative study. To avoid unrealistic mobility values, the channel doping was set to $N_\mathrm{A} = 1.25 \times 10^{18}\,\mathrm{cm}^{-3}$, electrically compensated by a similarly large donor doping $N_\mathrm{D}$. The simulation results in Fig. 3 show the same qualitative behavior as found in the $n^+$-$n$-$n^+$ structures. Altogether it was found that the SM model stays much closer to the MC results than the ET model, which makes the SM model a good choice for modeling sub-$100\,\mathrm{nm}$ devices.

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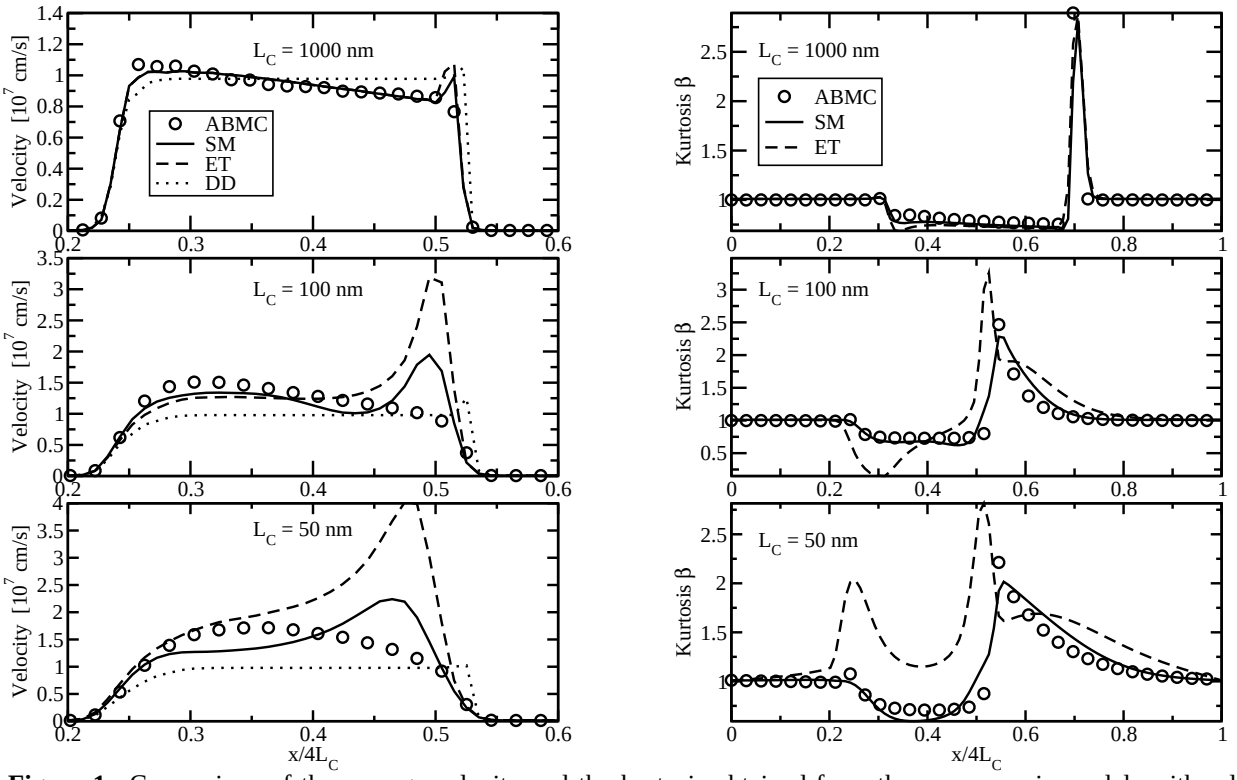


**Figure 1:** Comparison of the average velocity and the kurtosis obtained from the macroscopic models with self-consistent analytic-band MC (ABMC) simulations for three $n^+$-$n$-$n^+$ structures.

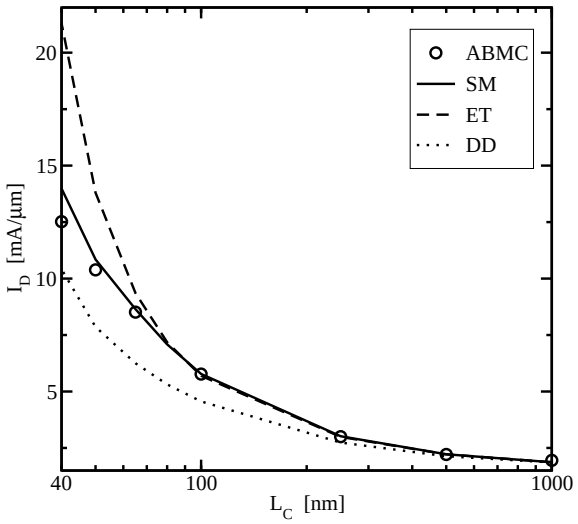


**Figure 2:** Comparison of the $n^+$-$n$-$n^+$ structure terminal currents obtained from the macroscopic models with self-consistent analytic-band MC (ABMC) simulations for various gate lengths.

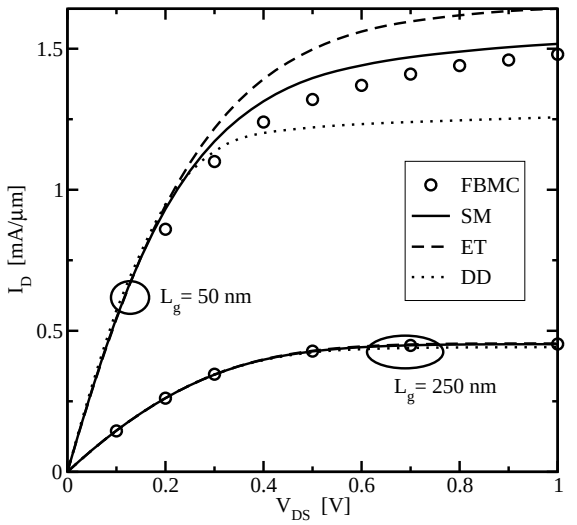


**Figure 3:** Comparison of the output characteristics obtained from the various models with self-consistent full-band Monte Carlo (FBMC) simulations for the $50\,\mathrm{nm}$ and $250\,\mathrm{nm}$ double-gate MOSFET.


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