# Investigation of Spurious Velocity Overshoot Using Monte Carlo Data

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**Abstract**

For the simulation of state-of-the-art devices hydrodynamic and energy transport models allow to account for non-local effects which cannot be captured by the drift-diffusion model. Although these models have been available for several decades, there are still unresolved issues. One of these issues is the occurrence of spurious peaks in the velocity profile which have originally been related to Bløtekjær's model. Recent research, however, showed that these peaks are inherent to both Stratton's and Bløtekjær's model. We investigate the origin of these peaks by introducing relaxation times, mobilities, and closure relations directly from a coupled Monte Carlo simulator. Although accurate modeling of the relaxation times and mobilities is important, it appears that the origin of the spurious peaks lies in the truncation of the infinite series of moments.

## 1 Introduction

In the traditional drift-diffusion (DD) approach the carrier energy is assumed to be in equilibrium with the electric field. Therefore, the DD model cannot predict non-local effects which occur in modern devices. Especially the overshoot in velocity is important to capture. Monte Carlo (MC) simulations predict an overshoot in the velocity when the electric field increases rapidly. This velocity overshoot can be qualitatively captured by higher order moment based models which, however, tend to overestimate this effect. Interestingly, these models also predict a velocity overshoot when the electric field decreases rapidly, e.g., at the end of a channel in a MOS transistor. This velocity overshoot is not observed in MC simulations and thus termed spurious velocity overshoot (SVO). Although the influence of this effect on device characteristics is probably not very dramatic, we feel that a thorough investigation of its cause is indeed important for the basic understanding of moment based models.

There has been an ongoing discussion in the literature on the cause of this effect. One of the first speculations was a weakness in the energy-transport (ET) model which is based on Bløtekjær's hydrodynamic model [1]. ET models and energy-balance (EB) models based on Stratton's approach [2] are closely related [1, 3], with the exception that the mobilities are defined in a different way. This leads to an additional driving term in the current relation of the EB model which is proportional to the spatial gradient of the mobility. This driving term can be reformulated and combined with the driving term of the temperature gradient yielding a modified prefactor of the temperature gradient. The modified prefactor is traditionally modeled as a constant and adjusted in such a way that the SVO is minimized [4]. It has already been pointed out that this approach is questionable [5], because the prefactor depends on the dominant scattering process which in turn depends on the doping and the applied voltages, and, therefore, no unique value can be found. Another important factor that has been attributed to SVO is the modeling of the mobilities which are not single valued functions of the energy [6]. As already argued by [7], SVO is not likely to be caused by the mobility alone.

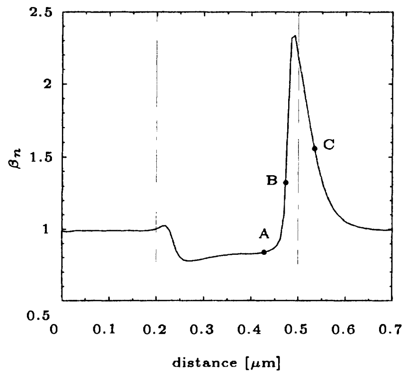


**Fig. 1:** Fourth order moment $\beta_n$ inside a $n^+$-$n$-$n^+$ test-structure

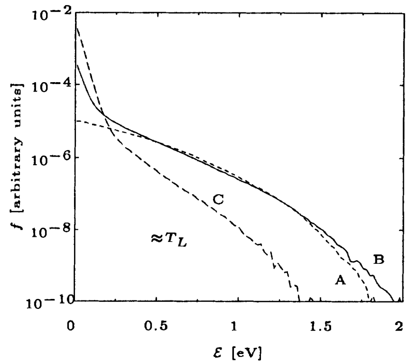


**Fig. 2:** Electron distribution functions inside a $n^+$-$n$-$n^+$ test-structure

## 2 Transport Models Coupled to Monte Carlo Simulator

A characteristic feature of moment based models is that the infinite hierarchy of moment equations has to be truncated to yield a finite number of equations. The highest order equation now contains a next higher moment which has to be modeled as a function of the lower order moments. Normally a heated Maxwellian shape is assumed for the distribution function (DF) which has the property that the fourth order moment $\langle \mathcal{E}^2 \rangle$ is proportional to the square of the average energy $\langle \mathcal{E} \rangle^2$. The accuracy of this relationship depends on the position in the device. To quantify the accuracy of this expression we define the kurtosis as [8]

$$\beta_n = \frac{3}{5} \frac{\langle \mathcal{E}^2 \rangle}{\langle \mathcal{E} \rangle^2} \tag{1}$$

which equals unity for a Maxwellian distribution and parabolic bands. A plot of $\beta_n$ inside an $n^+$-$n$-$n^+$ test-structure is given in Fig. 1 for a parabolic MC simulation. In the channel $\beta_n$ is in the range $[0.8, 1]$ and the error assumed by a Maxwellian closure is probably not too dramatic. However, when the hot channel carriers meet the large pool of cold carriers in the drain, $\beta_n$ reaches values above 2. Interestingly, this is exactly the region where the spurious velocity overshoot occurs. This is confirmed when we look at the distribution function at the points A, B, and C in Fig. 2 . For the channel point A, the curvature of the DF is smooth, reflected by a small value of $\beta_n$, whereas between the points B and C the contribution of the cold drain carriers increases while the high-energy tail relaxes slowly. Especially in these regions the Maxwellian shape which gives a straight line, is definitely a rather poor approximation.

To eliminate as many uncertainties as possible we use a parabolic ET model because non-parabolicity effects can only be approximately captured in the driving terms [9]. Furthermore we assume the validity of the diffusion approximation which allows to write the tensors as scalars and to neglect the contribution of the kinetic energy to the average carrier energy. These approximations are very common and will be reexamined later. In addition we restrict ourselves to the one-dimensional case, mainly because SVO is present in one-dimensional simulations and two-dimensional effects like real-space transfer further complicate any discussion. To remove the uncertainties in the relaxation time and mobility models we coupled our device simulator MINIMOS-NT to a MC simulator in a self-consistent manner where the potential distribution for the MC simulation was taken from the device simulator and the relaxation times for the device simulator from the last MC solution. A large number of scattering events had to be processed to achieve smooth relaxation times with small variance to obtain convergence within the moments models. In addition to the ET model we use our six moments model (SM) [8] for comparison which retains $\beta_n$ as a solution variable and introduces a closure for $\langle \mathcal{E}^3 \rangle$. Due to the existence of two carrier populations, the empirical closure we employed for $\langle \mathcal{E}^3 \rangle$ is most critical in the very same region as the closure for the four moments ET model [8].

## 3 Comparison

A comparison of simulated velocity profiles obtained from the ET and SM model with MC results is given in Fig. 3 which confirms that SVO is not caused by the mobility alone as the SVO spike is still observed using MC data for all relaxation times. However, the SM model improves the closure of the equation system which may be the reason for the reduced spike observed within the SM model.

To further investigate this effect, another set of simulations was performed using $\beta_n$ from the MC simulation to close the ET model, thus resulting in a correct closure of the four moments model. Furthermore, in one simulation the MC relaxation times were replaced by standard models, namely a constant energy relaxation time (0.33 ps), a simplified Hänsch mobility model [10]

$$\mu(T_n) = \frac{\mu_0}{1 + a(T_n - T_L)} \tag{2}$$

and a constant mobility ratio $\mu/\mu_S = 0.8$ where $\mu_S$ is the mobility of the energy flux [5].

$$\mathbf{S}_n = -\frac{5}{2}\frac{\mathrm{k_B^2}}{\mathrm{q}}\frac{\mu}{\mu_S}\Big(\nabla(nT_n^2\beta_n) + \frac{\mathrm{q}}{\mathrm{k_B}}\mathbf{E}nT_n\Big) \tag{3}$$

A comparison of these simulations with the MC values is given in Fig. 4. With the MC closure *and* the MC relaxation times the spike is completely removed whereas with the standard models it is quite pronounced, despite the correct closure. This leads us to the conclusion that SVO is a result of *both* the closure *and* the hysteresis in the relaxation times and can probably never be completely eliminated using a finite number of moment equations. However, as can be seen in Fig. 3, the error introduced by the closure is reduced when the number of moments is increased from four to six.

Fig. 4 serves as a good test for the approximations introduced in the derivation of the ET and SM model. Mainly, by employing the diffusion approximation, terms of the form $\langle \mathbf{u} \rangle \otimes \langle \mathbf{u} \rangle$ are neglected against $\langle \mathbf{u} \otimes \mathbf{u} \rangle$, one of the consequences being that the drift kinetic energy $m_\nu \langle \mathbf{u} \rangle^2/2$ is neglected against $\mathrm{k_B}T_n$. This contribution is only relevant as long as the carrier temperature is low and the velocity is high which is at the beginning of the channel in the velocity overshoot region. Indeed, a very small overestimation of the carrier temperature is observed in this region (Fig. 4). This contribution will gain more importance when the channel length is reduced. Fig. 4 stresses the importance of proper relaxation time and mobility models which influence the solution inside the whole device whereas the influence of the closure relation is strongest at the end of the channel and restricted to a relatively small region.

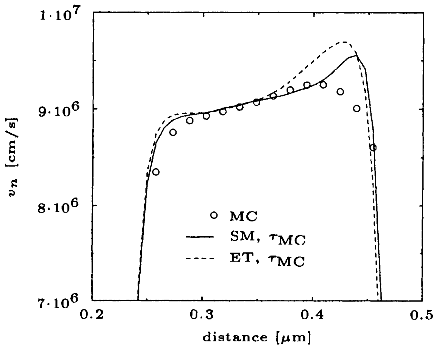


**Fig. 3:** Velocity profiles with MC relaxation times for the two transport models

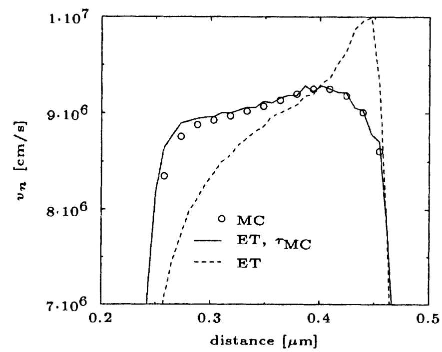


**Fig. 4:** Velocity profiles with MC relaxation times and closure

# 4 Conclusion

Spurious velocity overshoot has been attributed to several approximations introduced in the derivation of energy-transport models. We investigated the two most dominant effects which are caused by inaccuracies in the mobility and relaxation time models and by the truncation of the infinite series of moments. It has been demonstrated that accurate models for the mobilities and relaxation times are of utmost importance to reproduce velocity profiles inside the device. However, even with parameter values taken directly from Monte Carlo simulations, the spurious velocity overshoot remains in the velocity profiles but can be reduced by increasing the number of moments. This leads us to the conclusion that SVO is a result of both the closure and the inaccuracies in the physical models and can probably never be completely eliminated using a finite number of moments.


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