# On the Validity of the Relaxation Time Approximation for Macroscopic Transport Models

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**Abstract**

Although many doubts have been raised concerning its accuracy, the macroscopic relaxation time approximation is often used to approximate the weighted averages of the collision integral. More accurate approaches based on expansions of the distribution function deliver better results. Unfortunately these models depend on the fluxes of the system which causes a coupling of the flux relations. Our results indicate that this coupling requires accurate models for the energy tensors to obtain an overall quality improvement in the resulting transport model.

## 1 Introduction

Macroscopic transport models like the drift-diffusion (DD) model or the various hydrodynamic (HD) or energy-transport models can be derived from Boltzmann's equation by applying the method of moments [1]. Three approximations essentially determine the accuracy of these models: first, the equation system has to be truncated after a certain order $N$ to obtain a tractable equation set. Second, the tensors $\hat{\mathrm{U}}_i = \langle \mathbf{u} \otimes \mathbf{p}\, \mathcal{E}^{i-1} \rangle$ have to be approximated by the available moments which are the unknowns of the equation system, normally $n = \langle 1 \rangle$, $w_i = \langle \mathcal{E}^i \rangle$, and $\mathbf{V}_i = \langle \mathbf{u} \mathcal{E}^i \rangle$. And finally, the moments of the scattering operator $\mathbf{Q}_i$ have to be modeled properly. Since the scattering operator describes important physical properties of the system, this step is crucial. By expanding the distribution function into its moments the odd moments of the scattering integral $\mathbf{Q}_i$ can be written as functions of the odd moments $\mathbf{V}_i$ [2, 3, 4] and we obtain

$$\mathbf{Q}_i = -\left\langle \frac{\mathbf{p}\mathcal{E}^i}{\tau_{\mathbf{p}}} \right\rangle = \sum_{j=0}^{M} Z_{ij} \mathbf{V}_j \doteq -\mathrm{q}\, \hat{\mu}_i^{-1} \mathbf{V}_i \quad \text{with} \quad i = 0 \ldots M \,, \tag{1}$$

where $\tau_{\mathbf{p}}$ is the microscopic momentum relaxation time [5], the matrix $\hat{\mathrm{Z}}$ is determined by the scattering processes, $M = N/2 - 1$ is given by the order of the equation system, and $\hat{\mu}_i^{-1}$ is the inverse mobility tensor which in general depends on all even moments $w_i$ and all odd moments $\mathbf{V}_i$. An example of this type is the Hänsch mobility model [2]. Within the macroscopic relaxation time approximation the mobility tensor is assumed to be scalar and to depend only on the even moments $w_i$. Most commonly the mobilities are modeled as a function of the average energy $w_1$ only. In the following we will consider mobility data extracted from homogeneous bulk Monte Carlo simulations in

analogy to the model proposed in [6]. Strictly speaking, the relaxation time approximation is valid only under very stringent conditions which are definitely not fulfilled in modern deep-submicron devices [5, 7]. The failure of the relaxation time approximation to approximate the moments of the scattering integral is well documented [1].

## 2 Modeling of the Closure Relations

In the following we will model the closure relations for the tensors $\hat{\mathrm{U}}_i$ and the components of the scattering matrix $\hat{\mathrm{Z}}$ using an analytical distribution function model. It will be assumed that the distribution function can be obtained by displacing an isotropic distribution with a small energy-dependent displacement $\kappa\mathbf{K}(\mathcal{E}) = \kappa \sum_{j=0}^{M} \mathcal{E}^j \mathbf{K}_j$ where $\kappa$ is the Knudsen number. This displaced distribution will then be expanded up to second order. For the isotropic distribution we use a six moments description and a heated Maxwellian distribution [4]. With this distribution function model and Kane's nonparabolic dispersion relation the moments of the scattering integral $\mathbf{Q}_i$ obtained from Monte Carlo simulations can be well reproduced [4]. Another important property of this approach is that the tensors $\hat{\mathrm{U}}_i$ can be calculated up to second order. In particular, we obtain a zero-order scalar contribution $U_i$ that depends only on the even moments $w_i$ and a second-order contribution $\hat{\mathrm{U}}_i^{(2)}$ that also depends on the fluxes $\mathbf{V}_i$. For instance, for the simplest case of parabolic bands and a displaced Maxwellian distribution ($\mathbf{K} = \mathbf{K}_0 = m^*\mathbf{V}_0/\hbar$) we obtain the well-known expression $\hat{\mathrm{U}}_1 = (2/3)w_i\hat{\mathrm{I}} + \kappa^2 m^* \mathbf{V}_0 \otimes \mathbf{V}_0$. In general, the second-order term is a second-order polynomial in the fluxes $\mathbf{V}_i$. These second-order terms express the fact that the total energy of the electron gas is not equally distributed among the axes. This term is normally neglected in energy-transport models because it introduces hyperbolic modes into the equation system [1].

## 3 The Coupled Flux Relations

By taking the moments of Boltzmann's equation with the weight functions $\mathbf{p}\mathcal{E}^{\,i}$ we obtain general flux equations of the form $\mathbf{\Psi}_i = \mathbf{Q}_i$. With the driving force given by the electric field as $\mathbf{F} = -\mathrm{q}\mathbf{E}$, the fluxes $\mathbf{\Psi}_i$ are obtained as

$$\mathbf{\Psi}_i = -\hat{\mathrm{U}}_{i+1}\,\nabla \log \frac{1}{n} + \nabla \hat{\mathrm{U}}_{i+1} - \mathbf{F}(w_i\hat{\mathrm{I}} + i\hat{\mathrm{U}}_i) = \sum_{j=0}^{M} Z_{ij}\mathbf{V}_j \; . \tag{2}$$

We now invert these implicit relations to obtain explicit relations for the fluxes $\mathbf{V}_i$ as [4]

$$\mathbf{V}_i = \hat{\mu}_i \frac{\mathbf{F}}{\mathrm{q}} + \hat{\mathrm{D}}_i^n \nabla \log \frac{1}{n} - \sum_{j=0}^{M} Y_{ij} \nabla \hat{\mathrm{U}}_{j+1} \tag{3}$$

$$\text{with} \quad \hat{\mu}_i = -\mathrm{q} \sum_{j=0}^{M} Y_{ij}\,(w_j\hat{\mathrm{I}} + j\hat{\mathrm{U}}_j); \quad \hat{\mathrm{D}}_i^n = -\sum_{j=0}^{M} Y_{ij}\,\hat{\mathrm{U}}_{j+1}\;, \tag{4}$$

where the coefficients $Y_{ij}$ are the components of the matrix $\hat{\mathrm{Y}} = \hat{\mathrm{Z}}^{-1}$ which provide a coupling between the various flux equations (2). Within the relaxation time approximation there is no such coupling as the scattering tensor $\hat{\mathrm{Z}}$ reduces to a diagonal tensor with $Z_{ii} = -\mathrm{q}/\mu_i^{\mathrm{Bulk}}$.

## 4 Comparison

Evaluation of (4) using bulk Monte Carlo generated values for the moments $w_i$ gave an unexpected result which is in contradiction to the results published in [3] (cf. Fig. 1): When the second-order contributions to the tensors $\hat{\mathrm{U}}_i$ where neglected, the six moments model resulted in an error of $6\%$ in the average velocity $\mathbf{V}_0$ even though the scattering moments $\mathbf{Q}_i$ where accurate within $0.5\%$ (at $E = 50\,\mathrm{kV/cm}$). With included second-order contributions the accuracy of the average velocity was in the accuracy range of the scattering moments. A similar behavior was observed for the model based on the heated Maxwellian distribution but with a relatively large error at higher fields, independent of the order of truncation. The reason for this behavior is that for an electric field given by $\mathbf{E} = E\,\mathbf{e}_x$, the fluxes $\mathbf{V}_i$ are determined by the $xx$-component of the mobility tensors $\hat{\mu}_i$. Since for the coupled equation system these mobility tensors depend on all tensors $\hat{\mathrm{U}}_i$, the $xx$-component is significantly influenced by the second-order contribution to $\hat{\mathrm{U}}_i$. Note that this is not the case for models based on the relaxation time approximation where the average velocity $\mathbf{V}_0$ is independent of the tensors $\hat{\mathrm{U}}_i$. Therefore, by design, with homogeneous bulk mobility data these models exactly reproduce $\mathbf{V}_0$.

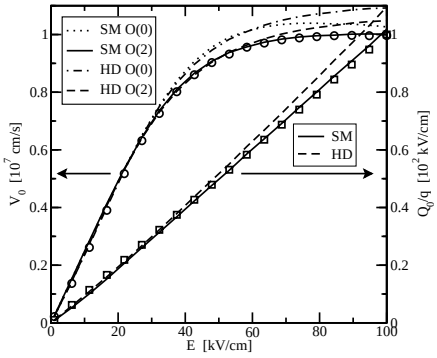


**Figure 1:** Comparison of $\mathbf{V}_0$ and $\mathbf{Q}_0$ from the six moments model (SM) and the Maxwellian model (HD) with Monte Carlo data (symbols).

To see how these models perform under inhomogeneous conditions we use one-dimensional cuts through the potential resulting from an ET transport solution of the $50\,\mathrm{nm}$ and $90\,\mathrm{nm}$ well-tempered MOSFETs [8] at $V_\mathrm{D} = V_\mathrm{G} = 1\,\mathrm{V}$. The resulting fluxes for both models are shown in Fig. 2. Whereas the rigorous model is accurate when the second-order contributions to the tensors $\hat{\mathrm{U}}_i$ are considered, a considerable error is introduced when they are neglected. The relaxation time approximation model, on the other hand, behaves the other way round and accurate results are only obtained when the second-order contributions to $\hat{\mathrm{U}}_i$ are neglected.

## 5 Conclusions

We arrive at the following conclusions: Even though the relaxation time approximation cannot properly reproduce the moments $\mathbf{Q}_i$ under inhomogeneous conditions, the errors in $\mathbf{Q}_i$ seem to compensate well with the errors in $\hat{\mathrm{U}}_i$ when the second-order contributions are neglected. Using the more rigorous model for $\mathbf{Q}_i$ based on the fluxes of the system requires highly accurate (and complicated) models for the second-order components of the tensors $\hat{\mathrm{U}}_i$, which is unlikely to reach the stability required for routine TCAD applications. Although this might not seem satisfactory from a theoretical point of view, relaxation time approximation based models employing tabulated or fitted homogeneous Monte Carlo results for $\mu_i^{\mathrm{Bulk}}(w_1)$ are a good compromise even for sub-$100\,\mathrm{nm}$ devices.

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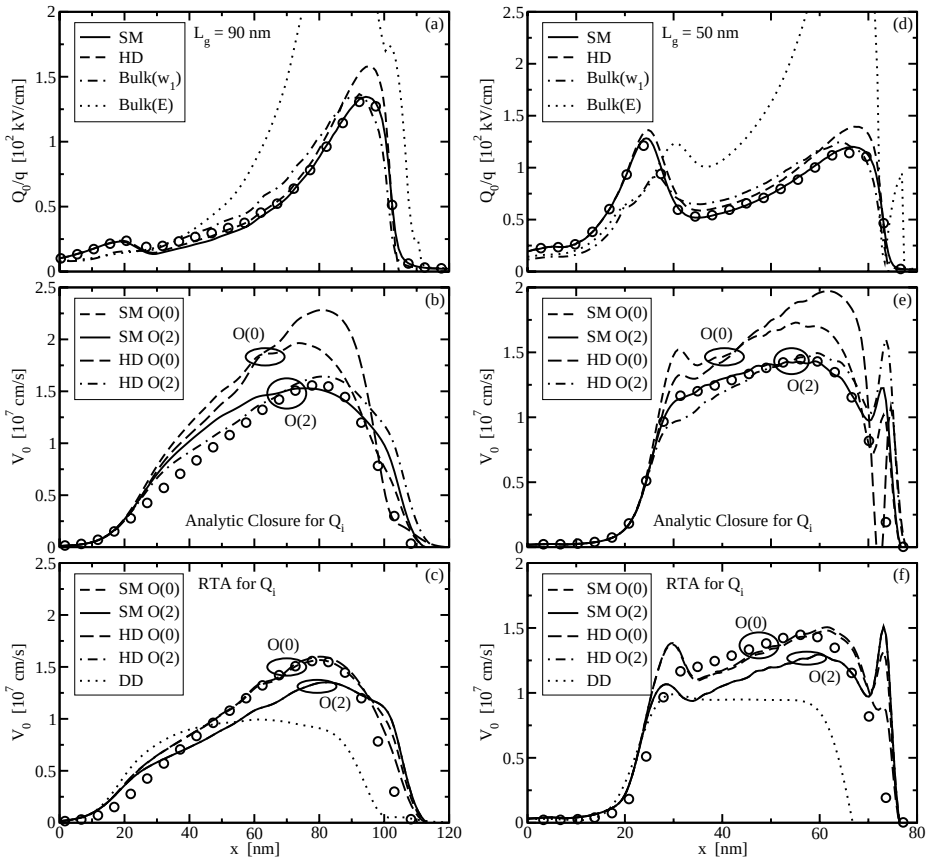


**Figure 2:** Comparison of the average velocity $\mathbf{V}_0$ and the first moment of the scattering integral $\mathbf{Q}_0$ predicted by the six moments model (SM) and the Maxwellian model (HD) with Monte Carlo data (symbols) for the two test MOSFETs. Note the good agreement of the second-order $\hat{\mathrm{U}}_i$ models plus analytical closure for $Q_i$ ($O(2)$) in Figs. (b) and (e) and of the zero-order $\hat{\mathrm{U}}_i$ models plus relaxation time approximation (RTA) $(O(0))$ in Figs. (c) and (f).