# On-/Off-State Design of Semiconductor Doping Profiles

Martin Burger* René Pinnau† Marie-Therese Wolfram‡

September 21, 2008

**Abstract**

We consider the multi-objective optimal dopant profiling of semiconductor devices. The two objectives are to gain a higher on-state current while the off-state current is kept small. This design question is treated as a constrained optimization problem, where the constraints are given by the stationary drift-diffusion model for the on-state and the linearized drift-diffusion model for the off-state. Using the doping profile as a state variable and the electrostatic potential as the new design variable, we obtain a simpler optimization problem, whose Karush-Kuhn-Tucker conditions partially decouple. Based on this observation we can construct a very efficient iterative optimization algorithm, which avoid to solve the fully coupled drift-diffusion system. Due to the simple structure of the adjoint equation, this algorithm can be easily included into existing semiconductor simulation tools. The efficiency and success of this multi-objective design approach is underlined by various numerical examples.

**Keywords:** Semiconductor design, drift-diffusion model, Gummel iteration, optimal control, multi-objective, dopant profiling.

**Subject Classification (AMS 2000):** 35J50, 49J20, 49K20.

## 1 Introduction

Optimal design problems for semiconductor devices recently received growing attention in modern microelectronics, and due to the ongoing miniaturization mathematical optimization methods play an increasingly important role (cf. e.g. [**?**, **?**, **?**, **?**, **?**, **?**, **?**]). The major goal of optimal semiconductor design is to improve the device characteristics, in particular current flows over some contact by designing a suitable device doping profile (representing the density of ion impurities within the material). In mathematical terms, this leads (at the coarsest level of device models) to a distributed optimal control problem for a system of partial differential equations, the so-called *drift-diffusion system*, in which the doping profile enters as a source term. The mathematical analysis and the construction of numerical optimization algorithms for the on-state design based on the drift-diffusion model is meanwhile in a mature state [**?**, **?**, **?**, **?**, **?**, **?**]. Recently, even extension to the the energy-transport model are available [**?**, **?**, **?**].

The aim of this paper is the numerical solution of optimal design problems which involve on- and off-states, i.e., a state with large applied voltage (on-state) and a second at equilibrium with possible voltage fluctuations (off-state) [**?**, **?**]. The typical design goal in such cases is to maximize the on-state current while keeping the off-state current (which can actually be a leakage current) small. By achieving this design goal, the practical performance of the device can be improved without increasing the losses when the device is switched off.

In the mathematical literature, there exist two different approaches to optimal dopant profiling, which differ in the respective choice of the design variable. Either, directly the doping profile is

*Institut für Numerische und Angewandte Mathematik, Westfälische Wilhelms-Universität Münster, Einsteinstr. 62, 48149 Münster, Germany (e-mail: martin.burger@uni-muenster.de)

†Fachbereich Mathematik, Universität Kaiserslautern, (e-mail: pinnau@mathematik.uni-kl.de)

‡Johann Radon Institute for Computational and Applied Mathematics (Austrian Academy of Sciences), Altenbergerstr. 69, 4040 Linz,Austria (e-mail: marietherese.wolfram@oeaw.ac.at)

used (cf. [?, ?, ?] and the references therein), or one uses the total charge density (cf. [?, ?] and the references therein). Here, we will follow the second one and extend the fast Gummel iteration for the on-state design presented in [?, ?] to the multi-objective on-/off-state design.

The paper is organized as follows. In the remainder of this section we introduce the underlying model equations for the optimal on-/off-state design of the doping profile, which is given by the stationary drift-diffusion model. The optimization is introduced and analyzed in Section 2. In particular, we suggest a linearized treatment of the off-state, we prove the existence of a minimizer and derive the first-order optimality system. A fast iterative procedure generalizing the classical Gummel iteration for the forward problem is introduced in Section 3. In Section 4, we present numerical results for the on-/off-state design of different semiconductor devices. Concluding remarks are given in Section 5.

## 1.1 The Drift-Diffusion Model

The stationary drift-diffusion system in physical variables consists of nonlinear elliptic equations for the electrostatic potential $V$, the electron density $n$, and the hole density $p$ [?, ?]:

$$\begin{aligned} \operatorname{div}(\epsilon_s \nabla V) &= q(n-p-C) && \text{in } \Omega, \\ \operatorname{div}(D_n \nabla n - \mu_n n \nabla V) &= 0 && \text{in } \Omega, \\ \operatorname{div}(D_p \nabla p + \mu_p p \nabla V) &= 0 && \text{in } \Omega, \end{aligned}$$

where $\epsilon_s$ denotes the semiconductor permittivity, $q$ the elementary charge, $\mu_n$ and $\mu_p$ are the electron and hole mobilities, $D_n$ and $D_p$ are the electron and hole diffusion coefficients, respectively. This is system is supplemented by homogeneous Neumann boundary condition on a part $\partial\Omega_N$ of the boundary, modeling the insulating parts of the boundary, and Dirichlet conditions on the remaining part, which models the Ohmic contacts of the device:

$$\begin{aligned} V(x) = V_D(x) = U(x) + V_{bi}(x) &= U(x) + U_T \ln\left(\frac{n_D(x)}{n_i}\right) && \text{on } \partial\Omega_D, \\ n(x) = n_D(x) &= \frac{1}{2}\left(C(x) + \sqrt{C(x)^2 + 4n_i^2}\right) && \text{on } \partial\Omega_D, \\ p(x) = p_D(x) &= \frac{1}{2}\left(-C(x) + \sqrt{C(x)^2 + 4n_i^2}\right) && \text{on } \partial\Omega_D. \end{aligned}$$

Here $n_i$ is the intrinsic density, $U_T$ the thermal voltage and $U$ is the applied biasing voltage.

Under usual conditions, the mobilities and diffusion coefficients are related by Einstein's relation, i.e., $D_{n/p} = \mu_{n/p} U_T$. which enables the transformation into the so-called *Slotboom variables* [?] defined by

$$n = n_i e^{-V/U_T} u, \qquad p = n_i e^{V/U_T} v. \tag{1.1}$$

The assumptions that $\epsilon_s$ and $q$ are constant allows for the choice of an appropriate scaling yielding the system

$$\lambda^2 \Delta V = \delta^2 (e^V u - e^{-V} v) - C \qquad \text{in } \Omega \tag{1.2a}$$

$$\operatorname{div}\left(\mu_n e^V \nabla u\right) = 0 \qquad \text{in } \Omega \tag{1.2b}$$

$$\operatorname{div}\left(\mu_p e^{-V} \nabla v\right) = 0 \qquad \text{in } \Omega \tag{1.2c}$$

where $\lambda^2 = (\epsilon_s U_T)/(q\, C_{\max} L^2)$ is the scaled Debye length of the device (for details see, e.g., [?]) and $\delta^2 = \frac{n_i}{C_{\max}}$. For brevity we shall use a scaling such that $\delta = 1$ in the subsequent presentation. For simplicity we shall use The Dirichlet boundary conditions can be written as

$$V = V_D = U + V_{bi} \qquad \text{on } \partial\Omega_D \tag{1.2d}$$

$$u = u_D \qquad \text{on } \partial\Omega_D \tag{1.2e}$$

$$v = v_D \qquad \text{on } \partial\Omega_D \tag{1.2f}$$

where $u_D$ and $v_D$ are the transformations of $n_D$ and $v_D$ under (1.1). On the remaining part $\partial\Omega_N = \partial\Omega \setminus \partial\Omega_D$, the homogeneous Neumann conditions can be formulated on $J_n$ and $J_p$, where $J_n$ and $J_p$ are the electron and hole current densities, which are related to the Slotboom variables by

$$J_n = \mu_n e^V \nabla u, \qquad J_p = -\mu_p e^{-V} \nabla v. \tag{1.2g}$$

Hence, we have

$$\frac{\partial V}{\partial \nu} = 0 \qquad \text{on } \partial\Omega_N \tag{1.2h}$$

$$\frac{\partial u}{\partial \nu} = 0 \qquad \text{on } \partial\Omega_N \tag{1.2i}$$

$$\frac{\partial v}{\partial \nu} = 0 \qquad \text{on } \partial\Omega_N \tag{1.2j}$$

Throughout the whole paper, we shall assume that all Dirichlet boundary values $V_D$, $u_D$, and $v_D$, are bounded in $H^{\frac{1}{2}}(\Omega) \cap L^\infty(\Omega)$, which is the basis for an existence proof of the drift-diffusion system in $(H^1(\Omega) \cap L^\infty(\Omega))^3$ [**?**].

# 2 The Optimal Design Problem

The design problem under investigation involves the on-state and the off-state of the device, i.e., we encounter a typical problem of multi-objective optimization. In general, one is interested in an increased on-state current while the off-state current is kept as small as possible. This allows for a better device performance in the on-state without increasing the so-called leakage-current in the off-state. Our optimization approach is essentially based on a combined least-squares formulation of both optimization goals.

One objective of the optimization, the on-state current flow over a contact $\Gamma$, is given by

$$I = \int_\Gamma J.d\nu = \int_\Gamma (J_n + J_p).d\nu, \tag{2.1}$$

where $J_n$ and $J_p$ are computed from the drift-diffusion model (1.2) for a specific onstate biasing voltage $U = U_{\text{on}}$.

Since the off-state is in general a fluctuation near the thermal equilibrium state (given for $U = 0$, where no current flows) and not exactl y known, we do not prescribe a specific offstate voltage $U_{\text{off}}$. Instead we intend to minimize the slope of the current voltage characteristics (IVC), i.e., we try to keep

$$K := \frac{dI}{dU}(0)$$

small, which actually suffices to guarantee small leakage currents. We shall see below that $K$ can be easily calculated from the linearized drift-diffusion model.

¡ This leads finally to the minimization of an objective functional of the form

$$Q(I, K) = Q_1(I) + \omega Q_2(K) \tag{2.2}$$

where $I$ and $K$ are defined via PDE constraints. Here, $\omega$ is a nonnegative weighting parameters, which allows for the adjustment of the two design goals.

## 2.1 On-State and Off-State

The on-state is clearly given by a solution of (1.2) for $U = U_{\text{on}}$ in (1.2d), from which we can directly compute $I$.

To compute the current slope $K$ we use a linearization around the thermal equilibrium state $(u_0, v_0, V_0)$ which is given by $u_0 = v_0 \equiv 1$ and

$$\lambda^2 \Delta V_0 = e^{V_0} - e^{-V_0} - C \qquad \text{in } \Omega \tag{2.3a}$$

$$V_0 = V_{bi} \qquad \text{on } \partial\Omega_D \tag{2.3b}$$

$$\frac{\partial V_0}{\partial \nu} = 0 \qquad \text{on } \partial\Omega_N. \tag{2.3c}$$

**Remark 2.1.** For an analytical discussion of the linearized drift-diffusion model we refer to [**?**, **?**] and the references therein. Note, that the nonlinear Poisson-Boltzmann equation allows for a unique weak solution.

Then, $K$ is calculated via

$$K = K_n + K_p, \quad K_n = e^{V_0} \nabla u_1, \quad K_p = -e^{-V_0} \nabla v_1, \tag{2.4}$$

where $u_1$ and $v_1$ are defined as the solutions of the carrier continuity equations

$$\operatorname{div}\left(e^{V_0} \nabla u_1\right) = 0 \qquad \text{in } \Omega \tag{2.5a}$$

$$\operatorname{div}\left(e^{-V_0} \nabla v_1\right) = 0 \qquad \text{in } \Omega, \tag{2.5b}$$

with boundary conditions

$$u_1 = -h, \quad v_1 = h \text{ on } \partial\Omega_D \tag{2.5c}$$

and

$$\frac{\partial u_1}{\partial \nu} = 0, \quad \frac{\partial v_1}{\partial \nu} = 0 \text{ on } \partial\Omega_N. \tag{2.5d}$$

**Remark 2.2.** Note that the system for the off-state fully decouples, which is one of the main ingredients for the construction of the upcoming iterative solution procedure. This is an effect of the special choice of the Slotboom variables. For the standard drift-diffusion model in the variables $(n, p, V)$ one would get a fully coupled system instead.

## 2.2 Design Goal and Stabilization

Typically, one is interested in an increase of the on-state outflow current $I$. This can be achieved by minimizing either

$$Q_1(I) = -I$$

or

$$Q_1(I) = \frac{1}{2}|I - I^*|^2, \tag{2.6}$$

where $I^*$ is some desired outflow current [**?**].

The easiest way to keep the off-state current small is to minimize

$$Q_2(K) = \frac{1}{2}K^2. \tag{2.7}$$

The standard design variable is the doping profile $C$. The adjoint approach, used in [**?**] yields satisfying results at moderate numerical costs. There, the optimization of the on-state current is done by a minimization of a functional of the form

$$Q_\beta(C) := Q(n(C), p(C), V(C)) + \frac{\beta}{2}\|C - C^*\|^2 \to \min_C, \tag{2.8}$$

where $C^*$ is a given doping profile .

A different approach for the on-state design was introduced in [**?**] and recently analytically investigated in [**?**]. There, the interpretations of control and state were exchanged between doping

profile $C$ and the potential $V$. Hence, the potential $V$ is used as the new design variable and the Poisson equation (1.2a) is interpreted as a state equation for the doping profile $C$.

In the following, we generalize this approach to our multi-objective design problem. Again, we introduce a new penalty term dependent on $V - V^*$ rather than on $C - C^*$. As the initial guess $V^*$ we use the one obtained from the solution of the on-state drift-diffusion system (1.2) with doping profile $C^*$. Since the Laplacian of $V - V^*$ is needed for the evaluation of $C - C^*$, it seems natural to use a penalty term dependent on the rescaled charge density

$$W := \Delta(V - V^*), \tag{2.9}$$

i.e., we intend to minimize the functional

$$Q_\epsilon(I, K, W) := Q(I, K) + \frac{\epsilon}{2} \int_\Omega |W(x)|^2 \, dx, \tag{2.10}$$

subject to (2.9), the on-state drift-diffusion system (1.2) and the off-state system (2.5). In order to ensure that $C$ does not change its boundary values, $W$ must satisfy homogeneous boundary conditions on $\partial\Omega_D$, on the remaining boundary we may use any homogeneous boundary condition. For simplicity we will carry out our analysis for

$$W = 0 \qquad \text{on } \partial\Omega. \tag{2.11}$$

Analogous treatment is possible for homogeneous Neumann conditions $\frac{\partial W}{\partial \nu} = 0$ on $\partial Omega_N$. The Neumann condition can be favourable with respect to implementation, since - as we shall see below - this will yield a Poisson equation for $W$ with the same type of boundary conditions as for $V$, hence the same solver can be used.

**Remark 2.3.** The numerical results in [**?**, **?**] show that the increase of the on-state current goes in general hand in hand with an increase of the off-state current. This is due to the fact that the higher on-state current is achieved by a larger doping concentration, resulting in more free carriers in the device. But this leads directly to an increase of the leakage current. Thus, a multi-objective design approach seems necessary. Note that our two design goals are competitive, which increases the numerical difficulties significantly.

## 2.3 Existence of a Minimizer

In the following we investigate analytically the optimization problem

$$Q_\epsilon(I, K, W) \to \min_{(u,v,u_1,v_1,V,V_0,W)\in\mathcal{D}_{ad}}, \tag{2.12}$$

with the admissible domain

$$\mathcal{D}_{ad} := \{(u, v, u_1, v_1, V, V_0, W) \in H^1(\Omega)^4 \times (H^1(\Omega) \cap L^\infty(\Omega))^2 \times L^2(\Omega) \\ \text{satisfying (1.2b)-(1.2j), (2.5), (2.3), (2.9) }\}.$$

**Theorem 2.4** (Existence)**.** *Let $\epsilon > 0$ be given. Then there exists a minimizer*

$$(\overline{u}, \overline{v}, \overline{u}_1, \overline{v}_1, \overline{V}, \overline{V}_0, \overline{W}) \in H^1(\Omega)^4 \times (H^1(\Omega) \cap L^\infty(\Omega))^2 \times L^2(\Omega) \tag{2.13}$$

*of the constrained minimization problem* (2.12)*.*

**Proof.** Suppose $(u^k, v^k, u_1^k, v_1^k, V^k, V_0^k, W^k)_{k\in\mathbb{N}}$ is a minimizing sequence, then the coercivity of $Q_\epsilon$ with respect to $W$ ensures that $(W^k)_{k\in\mathbb{N}}$ is uniformly bounded in $L^2(\Omega)$.

Thus, by standard elliptic regularity [**?**], $(V^k - V^*)_{k\in\mathbb{N}}$ is uniformly bounded in $H^2(\Omega) \hookrightarrow C(\overline{\Omega})$. Since the a-priori guess $V^*$ is in $L^\infty(\Omega)$, we obtain uniform boundedness of $(V^k)_{k\in\mathbb{N}}$ in $L^\infty(\Omega)$. Standard energy arguments for the elliptic equations (1.2b) and (1.2c) consequently yield the boundedness of $(u^k)_{k\in\mathbb{N}}$ and $(v^k)_{k\in\mathbb{N}}$ in $H^1(\Omega) \cap L^\infty(\Omega)$.

From

$$C = C^* - \lambda^2 W + e^V u - e^{V^*} u^* - e^{-V} v + e^{-V^*} v^*$$

we get, using (2.3a),

$$\lambda^2 \Delta V_0^k = e^{V_0^k} - e^{-V_0^k} - \left( C^* - \lambda^2 W^k + e^{V^k} u^k - e^{V^*} u^* - e^{-V^k} v^k + e^{-V^*} v^* \right) \tag{2.14}$$

This monotone equation admits a unique solution $V_0^k \in H^1(\Omega) \cap L^\infty(\Omega)$, which depends Lipschitz continuously on the right-hand side [**?**, Lemma 3.3.14]. Thus, also $(V_0^k)_{k\in\mathbb{N}}$ is uniformly bounded in $H^1(\Omega) \cap L^\infty(\Omega)$.

Again, standard estimates for the elliptic equations (2.5) yield the boundedness of $(u_1^k)_{k\in\mathbb{N}}$ and $(v_1^k)_{k\in\mathbb{N}}$ in $H^1(\Omega) \cap L^\infty(\Omega)$.

Thus, we can extract a weakly converging subsequence, again denoted by

$$(u^k, v^k, u_1^k, v_1^k, V^k, V_0^k, W^k)_{k\in\mathbb{N}} \in H^1(\Omega)^4 \times H^1(\Omega)^2 \times L^2(\Omega),$$

which also preserves the $L^\infty$ bound (and such that $\Delta(V^k - V^*)$ converges weakly in $L^2(\Omega)$). The weak closedness of the admissible domain and the weak lower semicontinuity of the objective functional imply that the weak limit of this subsequence is a minimizer of (2.12). □

## 2.4 First-Order Optimality

For the following analysis it is most convenient to eliminate $C$ in (2.3a) by (1.2a) and to introduce the new variable $\psi = V_0 - V$. This yields the equation

$$\lambda^2 \Delta \psi = e^V \left( e^\psi - u \right) - e^{-V} \left( e^{-\psi} - v \right) \qquad \text{in } \Omega \tag{2.15}$$

$$\psi = -U \qquad \text{on } \partial\Omega_D \tag{2.16}$$

$$\frac{\partial \psi}{\partial \nu} = 0 \qquad \text{on } \partial\Omega_N. \tag{2.17}$$

For notational convenience we define the vector of state variables $y := (u, v, u_1, v_1, V, \psi)$ and the vector of Lagrange multipliers $\mu := (\mu_1, \mu_2, \mu_3, \mu_4, \mu_5, \mu_6)$. In order to derive the first-order optimality conditions, we define the Lagrangian $\mathcal{L} : \mathcal{D}_{ad} \times H^1(\Omega)^6 \to \mathbb{R}$ given by

$$\begin{aligned}
\mathcal{L}(y, W; \mu) := Q_\epsilon(I(y, W), K(y, W)) &+ \int_\Omega \left( e^V \nabla u \nabla \mu_1 - e^{-V} \nabla v \nabla \mu_2 \right) \, dx \\
&+ \int_\Omega \left( e^{V+\psi} \nabla u_1 \nabla \mu_3 - e^{-(V+\psi)} \nabla v_1 \nabla \mu_4 \right) \, dx \\
&+ \lambda^2 \int_\Omega \nabla \psi \nabla \mu_5 + \left[ e^V \left( e^\psi - u \right) - e^{-V} \left( e^{-\psi} - v \right) \right] \mu_5 \, dx \\
&+ \int_\Omega \left( \nabla (V - V^*) \nabla \mu_6 + W \mu_6 \right) \, dx.
\end{aligned} \tag{2.18}$$

Due to $V, \psi \in H^1(\Omega) \cap L^\infty(\Omega)$ and $(u, v) \in H^1(\Omega)^2$ one can easily verify Fréchet-differentiability of $\mathcal{L}$.

**Proposition 2.5.** *The Lagrangian $\mathcal{L}$ is continuously Fréchet-differentiable on $\mathcal{D}_{ad} \times H^1(\Omega)^6$.*

Each solution of the optimization problem is a saddle point of the Lagrangian, i.e., a solution of

$$\inf_{(y,W)} \sup_\mu \mathcal{L}(y, W, \mu). \tag{2.19}$$

For such saddle-points we can derive the Karush-Kuhn-Tucker conditions by computing the variations of the Lagrangian $\mathcal{L}$ with respect to the primal and dual variables, which all must vanish.

The variations with respect to the dual variables just yield the equality constraints, while from the variation with respect to the primal variables we deduce that

$$
\begin{aligned}
0 &= \frac{\partial}{\partial u} Q_\epsilon(y,W)\hat{u} + \int_\Omega e^V \nabla\hat{u}.\nabla\mu_1 dx + \int_\Omega \hat{u} e^V \mu_5 dx && (2.20a)\\
0 &= \frac{\partial}{\partial v} Q_\epsilon(y,W)\hat{v} - \int_\Omega e^{-V} \nabla\hat{v}.\nabla\mu_2 dx + \int_\Omega \hat{v} e^{-V} \mu_5 dx && (2.20b)\\
0 &= \frac{\partial}{\partial u_1} Q_\epsilon(y,W)\hat{u}_1 + \int_\Omega \left(e^{V+\psi}\nabla\hat{u}_1.\nabla\mu_3\right) dx && (2.20c)\\
0 &= \frac{\partial}{\partial v_1} Q_\epsilon(y,W)\hat{v}_1 - \int_\Omega \left(e^{-(V+\psi)}\nabla\hat{v}_1.\nabla\mu_4\right) dx && (2.20d)\\
0 &= \frac{\partial}{\partial \psi} Q_\epsilon(y,W)\hat{\psi} + \int_\Omega \hat{\psi}\left(e^{V+\psi}\nabla u_1.\nabla\mu_3 - e^{-(V+\psi)}\nabla v_1\nabla\mu_4\right) dx \\
&\quad + \int_\Omega \lambda^2\nabla\hat{\psi}.\nabla\mu_5 + \hat{\psi}\left(e^{V+\psi} + e^{-(V+\psi)}\right)\mu_5 dx && (2.20e)\\
0 &= \frac{\partial}{\partial V} Q_\epsilon(y,W)\hat{V} + \int_\Omega \hat{V}\left(e^V\nabla u.\nabla\mu_1 + e^{-V}\nabla v\nabla\mu_2\right) + \nabla\hat{V}.\nabla\mu_6 dx \\
&\quad + \int_\Omega \hat{V}\left(e^{V+\psi}\nabla u_1\nabla\mu_3 - e^{-(V+\psi)}\nabla v_1\nabla\mu_4\right) dx \\
&\quad + \int_\Omega \hat{V}\left(e^V\left(e^\psi - u\right) - e^{-V}\left(e^{-\psi} - v\right)\right)\mu_5 dx && (2.20f)\\
0 &= \int_\Omega \hat{W}(\epsilon W + \mu_6) dx, && (2.20g)
\end{aligned}
$$

holds for all variations $(\hat{u},\hat{v},\hat{u}_1,\hat{v}_1,\hat{V},\hat{\psi},\hat{W}) \in H^1(\Omega)^6 \times L^2(\Omega)$.

Note that the so-called *adjoint system* (2.20) has a simple triangular structure with respect to the Lagrangian variables $\mu$. For given primal variables $y$ we can solve consecutively for $\mu_3, \mu_4$ followed by $\mu_5$ and $\mu_1, \mu_2$ and finally $\mu_6$. Thus, the problem of proving existence and uniqueness of Lagrangian variables $\mu \in H^1_{0,D}(\Omega)^6$ solving (2.20) for given primal variables $y$, simplifies to analyzing subsequently six different linear variational problems, which turn out to be coercive (compare also the existence proof in [**?**]).

**Theorem 2.6.** *Let $(y,W) \in \mathcal{D}_{ad}$ be given, then there exists a unique solution $\mu \in H^1_{0,D}(\Omega)^6$ of the variational problem* (2.20).

**Remark 2.7.** This yields another advantage of our approach with respect to the direct optimal control approach, where analyzing the adjoint problem is a difficult task, which is possible only close to thermal equilibrium (cf. [**?**]), in general existence of Lagrange multipliers is not guaranteed.

To derive the strong form the adjoint equations we proceed by computing the partial derivatives of $Q_\epsilon$. We get

$$Q_1'(u,v,V)(\hat{u},\hat{v},\hat{V}) = (I - I^*)\int_\Gamma \left(e^V\frac{\partial\hat{u}}{\partial\nu} - e^{-V}\frac{\partial\hat{v}}{\partial\nu}\right) ds \tag{2.21}$$

and

$$Q_2'(u_1,v_2,\psi)(\hat{u}_1,\hat{v}_1,\hat{\psi}) = K\int_\Gamma \left(e^{V+\psi}\frac{\partial\hat{u}_1}{\partial\nu} - e^{-(V+\psi)}\frac{\partial\hat{v}_1}{\partial\nu}\right) ds \tag{2.22}$$

If we choose the Lagrangian variables $\mu_i$, $i = 1,2$ such that $\mu_i = 0$ only on $\partial\Omega_D \setminus \Gamma$ and $\mu_1 = \mu_2 = \eta$ on $\Gamma$ for some real constant $\eta$, then we can derive a simple form of the optimality

system. With this choice, the Lagrangian becomes

$$\begin{aligned}\mathcal{L}(y,W;\mu) = Q_\epsilon(I(y,W),K(y,W)) &+ \int_\Omega \left(e^V \nabla u \nabla \mu_1 - e^{-V}\nabla v \nabla \mu_2\right)\ dx \\ &+ \int_\Omega \left(e^{V+\psi}\nabla u_1 \nabla \mu_3 - e^{-(V+\psi)}\nabla v_1 \nabla \mu_4\right)\ dx \\ &+ \lambda^2 \int_\Omega \nabla\psi\nabla\mu_5 + \left[e^V\left(e^\psi - u\right) - e^{-V}\left(e^{-\psi}-v\right)\right]\mu_5\ dx \\ &+ \int_\Omega \left(\nabla(V-V^*)\nabla\mu_6 + W\mu_6\right)\ dx - \eta I. \end{aligned} \tag{2.23}$$

and the optimality with respect to $u$ yields

$$(I - I^* - \eta)\int_\Gamma \left(e^V \frac{\partial \hat{u}}{\partial \nu}\right) ds + \int_\Omega \left(e^V \nabla \hat{u}.\nabla\mu_1\right) dx + \int_\Omega \hat{u} e^V \mu_5 dx = 0. \tag{2.24}$$

With the choice $\eta = I - I^*$, this reduces to the weak formulation corresponding to the elliptic partial differential equation

$$\operatorname{div}\left(e^V \nabla \mu_1\right) = -e^V \mu_5 \qquad \text{in } \Omega, \tag{2.25a}$$

subject to the boundary conditions

$$\begin{aligned} \mu_1 &= I - I^* \qquad \text{on } \Gamma && (2.25b)\\ \mu_1 &= 0 \qquad \text{on } \partial\Omega_D \setminus \Gamma && (2.25c)\\ \frac{\partial \mu_1}{\partial \nu} &= 0 \qquad \text{on } \partial\Omega_N. && (2.25d)\end{aligned}$$

Analogous reasoning yields the equation

$$\operatorname{div}\left(e^{-V} \nabla \mu_2\right) = -e^{-V} \mu_5 \qquad \text{in } \Omega, \tag{2.26a}$$

subject to the boundary conditions

$$\begin{aligned} \mu_2 &= -(I - I^*) \qquad \text{on } \Gamma && (2.26b)\\ \mu_2 &= 0 \qquad \text{on } \partial\Omega_D \setminus \Gamma && (2.26c)\\ \frac{\partial \mu_2}{\partial \nu} &= 0 \qquad \text{on } \partial\Omega_N. && (2.26d)\end{aligned}$$

Next, we choose the Lagrangian variables $\mu_i$, $i = 3, 4$ such that $\mu_i = 0$ only on $\partial\Omega_D \setminus \Gamma$ and $\mu_3 = \mu_4 = \eta$ on $\Gamma$ for some real constant $\rho$. With this choice, the Lagrangian becomes

$$\begin{aligned}\mathcal{L}(y,W;\mu) = Q_\epsilon(I(y,W),K(y,W)) &+ \int_\Omega \left(e^V \nabla u \nabla \mu_1 - e^{-V}\nabla v \nabla \mu_2\right)\ dx \\ &+ \int_\Omega \left(e^{V+\psi}\nabla u_1 \nabla \mu_3 - e^{-(V+\psi)}\nabla v_1 \nabla \mu_4\right)\ dx \\ &+ \lambda^2 \int_\Omega \nabla\psi\nabla\mu_5 + \left[e^V\left(e^\psi - u\right) - e^{-V}\left(e^{-\psi}-v\right)\right]\mu_5\ dx \\ &+ \int_\Omega \left(\nabla(V-V^*)\nabla\mu_6 + W\mu_6\right)\ dx - \rho K. \end{aligned} \tag{2.27}$$

and the optimality with respect to $u_1$ yields

$$(K - \rho)\int_\Gamma \left(e^{V+\psi} \frac{\partial \hat{u}_1}{\partial \nu}\right) ds + \int_\Omega \left(e^{V+\psi} \nabla \hat{u}_1.\nabla\mu_3\right) dx = 0. \tag{2.28}$$

With the choice $\rho = K$, this reduces to the weak formulation of

$$\operatorname{div}\left(e^{V+\psi} \nabla \mu_3\right) = 0 \qquad \text{in } \Omega, \tag{2.29a}$$

subject to the boundary conditions

$$\begin{aligned} \mu_3 &= K \qquad \text{on } \Gamma && (2.29b)\\ \mu_3 &= 0 \qquad \text{on } \partial\Omega_D \setminus \Gamma && (2.29c)\\ \frac{\partial \mu_3}{\partial \nu} &= 0 \qquad \text{on } \partial\Omega_N. && (2.29d) \end{aligned}$$

Repeating the argument we get the equation

$$\operatorname{div}\left(e^{-(V+\psi)}\nabla\mu_4\right) = 0 \qquad \text{in } \Omega, \tag{2.30a}$$

subject to the boundary conditions

$$\begin{aligned} \mu_4 &= -K \qquad \text{on } \Gamma && (2.30b)\\ \mu_4 &= 0 \qquad \text{on } \partial\Omega_D \setminus \Gamma && (2.30c)\\ \frac{\partial \mu_4}{\partial \nu} &= 0 \qquad \text{on } \partial\Omega_N. && (2.30d) \end{aligned}$$

Further, the optimality with respect to $\psi$ is the variational formulation of the elliptic equation

$$-\lambda^2\Delta\mu_5 + \left(e^{V+\psi} + e^{-(V+\psi)}\right)\mu_5 = -K_n\cdot\nabla\mu_3 - K_p\cdot\nabla\mu_4 \qquad \text{in } \Omega, \tag{2.31a}$$

subject to the boundary conditions

$$\begin{aligned} \mu_5 &= 0 \qquad \text{on } \partial\Omega_D && (2.31b)\\ \frac{\partial \mu_5}{\partial \nu} &= 0 \qquad \text{on } \partial\Omega_N. && (2.31c) \end{aligned}$$

The optimality with respect to $V$ is the variational formulation of the elliptic equation

$$\begin{aligned} -\Delta\mu_6 + \left(e^V(e^\psi - u) + e^{-V}(e^{-\psi} - v)\right)\mu_5 &= \\ -K_n\cdot\nabla\mu_3 - K_p\cdot\nabla\mu_4 - J_n\nabla\mu_1 - J_p\nabla\mu_2 &\qquad \text{in } \Omega, \end{aligned} \tag{2.32a}$$

subject to the boundary conditions

$$\begin{aligned} \mu_6 &= 0 \qquad \text{on } \partial\Omega_D && (2.32b)\\ \frac{\partial \mu_6}{\partial \nu} &= 0 \qquad \text{on } \partial\Omega_N. && (2.32c) \end{aligned}$$

Finally, we determine the optimality condition with respect to $W$ which can be rewritten as the equation

$$\epsilon W = \mu_6 \qquad \text{in } \Omega. \tag{2.33}$$

**Remark 2.8.** The simple form of (2.33) allows for the elimination of the adjoint variable $\mu_6$.

# 3 The Generalized Gummel Iteration

In the following we present an iterative procedure motivated by the classical Gummel iteration for the solution of the drift diffusion model [**?**]. This results in a full decoupling of the KKT systems, such that only a sequence of elliptic equations needs to be solved. This approach was already successfully used for the on-state design in [**?**] and analytically investigated in [**?**].

Standard techniques for the computation of a minimizer of (2.12), like gradient descent or Newton's method for the KKT system (2.20), require the consecutive solution of the state and of the adjoint system, which is in general non-elliptic due to the strong influence of first-order terms. Further, suitable updates for the design variable are needed (compare [**?**, **?**]).

Instead, we exploit the triangular structure of the adjoint system and use a lower triangular approximation of the optimality system: We first solve equation (2.9) with given $W$ for the potential $V$, and subsequently the continuity equations (1.2b), (1.2c) with given potential $V$ for $u$ and $v$. Using this data we can solve (2.15) for the linearized potential $\psi$ followed by the solution of (2.5) for $u_1$ and $v_1$. With given state variables, we solve the adjoint equations (2.29a), (2.30a) to obtain the Lagrangian variables $\mu_3$ and $\mu_4$. Then we can solve (2.31a) for $\mu_5$, followed by the solution of (2.25a), (2.26a) for $\mu_1$ and $\mu_2$. Finally, we can compute $\mu_6$ from (2.32a) and update $W$ via (2.33).

All together, we can write this iteration as

**Algorithm 3.1.**

1. Choose $W^0$.
2. For $k = 1, 2, \ldots$ solve consecutively

$$\begin{aligned}
\Delta V^k &= \Delta V^* + W^{k-1} \\
\operatorname{div}\,(e^{V^k}\nabla u^k) &= 0 \\
\operatorname{div}\,(e^{-V^k}\nabla v^k) &= 0
\end{aligned}$$

$$\begin{aligned}
\lambda^2 \Delta\psi^k &= e^{V^k}\left(e^{\psi^k} - u^k\right) - e^{-V^k}\left(e^{-\psi^k} - v^k\right) \\
\operatorname{div}\,(e^{V^k+\psi^k}\nabla u_1^k) &= 0 \\
\operatorname{div}\,(e^{-(V^k+\psi^k)}\nabla v_1^k) &= 0
\end{aligned}$$

$$\begin{aligned}
\operatorname{div}\,(e^{V^k+\psi^k}\nabla \mu_3^k) &= 0 \\
\operatorname{div}\,(e^{-(V^k+\psi^k)}\nabla \mu_4^k) &= 0 \\
-\lambda^2\Delta\mu_5^k + \left(e^{V^k+\psi^k} + e^{-(V^k+\psi^k)}\right)\mu_5^k &= -K_n^k\cdot\nabla\mu_3^k - K_p^k\cdot\nabla\mu_4^k
\end{aligned}$$

$$\begin{aligned}
\operatorname{div}\,(e^{V^k}\nabla\mu_1^k) &= e^{V^k}\mu_5^k \\
\operatorname{div}\,(e^{-V^k}\nabla\mu_2^k) &= -e^{-V^k}\mu_5^k
\end{aligned}$$

$$\begin{aligned}
-\Delta\mu_6^k + \left(e^{V^k}(e^{\psi^k} - u^k) + e^{-V^k}(e^{-\psi^k} - v^k)\right)\mu_6^k &= \\
&= -K_n^k\cdot\nabla\mu_3^k - K_p^k\cdot\nabla\mu_4^k - J_n^k\nabla\mu_1^k - J_p^k\nabla\mu_2^k \\
\epsilon W^k &= \mu_6^k
\end{aligned}$$

subject to the above boundary conditions.

With this generalized Gummel iteration we mainly need to solve linear Poisson and continuity equations and hence can use all building blocks of typical device simulators. The only nonlinear equation is the third one for $\psi^k$, which is actually a Poisson-Boltzmann equation in equilibrium and can be solved efficiently via a Newton iteration.

**Remark 3.2.** The corresponding value of the doping profile can be computed independently by

$$C^k - C^* = -\lambda^2 W^k + n^k - n^* - p^k + p^*, \tag{3.1}$$

where $n^k = e^{V^k}u^k$ and $p^k = e^{-V^k}v^k$.