

MATHEMATICS CLINIC



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Gate to Base Capacitance Modeling for Nano-scale MOSFETs

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1. Introduction

The continuing down-scaling of CMOS technology has brought serious deterioration in the accuracy of the SPICE(simulation program with integrated circuit emphasis) device models used in the design of chip functions. This is due to in part to quantum effects that occur in modern nano-scale MOSFET devices. The focus of this paper is on modeling the quantum effects based on the Density-Gradient (DG) model. In [AFY06], a first integral to the Density Gradient Equations was determined for the MOSFET under Inversion. In [CUA07], asymptotic expansions for the inversion region were calculated. In this report the parallel results for the Accumulation Region will be determined. This paper focuses on modeling the capacitance from the gate to the base as a function of the applied voltage.

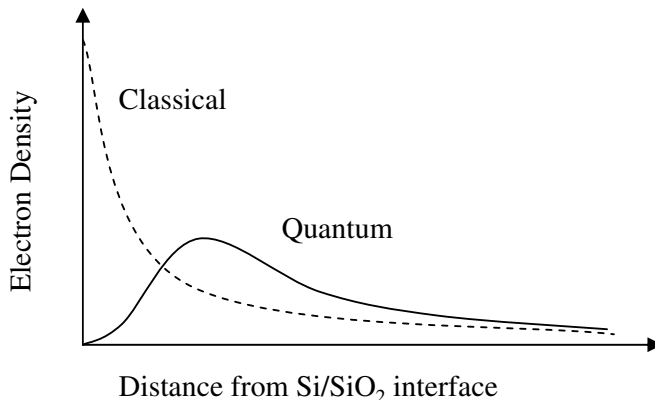


Figure 1: Comparison of classical and quantum solutions for the electron density.

A full treatment using quantum mechanics requires QM solutions in the gate metal material and in the oxide insulator, as well as in the silicon base. The oxide, having a large barrier height, would generate only a small electron density. In this case the electrons are said to have leaked or tunnelled into the oxide. In the treatment here, the electron density in the insulator is taken to be zero. The quantum treatment requires that the electron density be continuous so that the boundary condition at the oxide/silicon interface is zero electron density, whereas the classical theory based on the drift-diffusion model using the quasi 1-D approximation gives maximum charge density at this interface. This is the main discrepancy between the classical and quantum models. Several models have received attention. Full solutions of the Schrödinger and Gauss equations, and various other approximations, all require high level numerical simulations. This multi-dimensional microscopic solution is inappropriate for practical circuit application [AT87, BRYDA98].

The classical description, which is conventionally the drift-diffusion (DD) current density model, may be obtained by assuming that the internal energy densities of the electron and hole gases have a logarithmic dependence on the charge densities. A more general series expansion of the density using the kinetic theory of gases gives that the energy depends not only on the density but also on the spatial gradient of gas density [AT87, AYLDV97]. This is the central assumption of the DG theory and it is derived from electron and hole kinetics by applying hydrodynamic theory. The association with quantum mechanical effects is made by interpreting the extra DG term as a quantum term, and suitably changing the boundary conditions. However, the DG model may also be generated directly from the quantum mechanics for electrons by expressing the Schrödinger wave function in amplitude/phase form (see section 2.2 of [CUA07]). The DG model has been solved numerically for a variety of devices and it has shown good accuracy compared with more complete models, in particular with quantum microscopic solutions for tunneling and confinement effects; see [AT87, p. 7964], [An90, p. 1228] and [AI89 p. 9537].

The quantum term in the DG model is higher order than the DD terms and it is multiplied by a numerically small factor. This indicates a boundary layer behavior which is confirmed by the numerical results: the inversion charge density is reduced significantly in a small layer close to the silicon/silicon-oxide interface, but the charge behavior outside this layer is similar to the non-quantum, classical solution (see Figure 1). The maximum of the classical charge distribution is shifted away from the oxide interface under the influence of quantum effects, and its value may be reduced by up to two orders of magnitude. This loss of electrons results in diminished source-to-drain current, and it affects the gate capacitance circuit element. (The shift in the maximum density may be viewed as an increased oxide thickness.) Also, in the case when the electron mobility is position dependent, an effective value is obtained by averaging with respect to the charge carrier density, and this value is amended due to the classical to quantum profile change shown in Figure 1.

In this paper the approach is to find analytic solutions to the DG model for the capacitance and then test these solutions against the numeric solutions. Figure 2 shows the change in capacitance between the drift diffusion model and the density gradient model. This difference found in the accumulation and inversion regions is of most interest. Ultimately, a good blend throughout all three regions is the aim. In general the results for one region will be done explicitly and the parallel result will be stated.

2. Model Equations and Parameter Scaling

2.1 The Drift-Diffusion Equations. The motion of electrons and holes is assumed to be governed both by the electric field and by diffusion using the standard Fick's law. This gives for the electron and hole fluxes

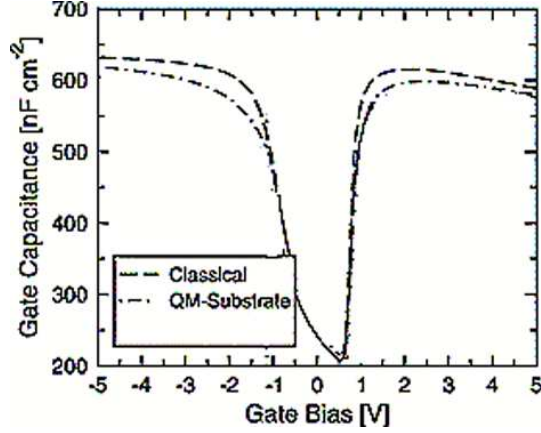


Figure 2: Comparison of classical and quantum solutions for the capacitance.

$$\left. \begin{aligned} \mathbf{J}_n &= q(n\mu_n\mathbf{E} + D_n\nabla n) \\ \mathbf{J}_p &= q(p\mu_p\mathbf{E} - D_p\nabla p) \end{aligned} \right\} \quad (2.1)$$

where $\mathbf{J}_n, \mathbf{J}_p$ are the electron and hole current densities, q is the magnitude of the electronic charge, n, p are the electron and hole concentrations and D_n, D_p are the electron and hole diffusivities. The electron hole mobilities μ_n and μ_p depend in general on doping levels and the electrostatic field \mathbf{E} , but usually are taken as constant. With the Einstein relation:

$$D = \frac{kT\mu}{q} \quad (2.2)$$

and with

$$\mathbf{E} = -\nabla\psi \quad (2.3)$$

we can write

$$\left. \begin{aligned} \mathbf{J}_n &= n\mu_n\nabla(-\psi q + kT \ln n) = -qn\mu_n\nabla\Phi_n \\ \mathbf{J}_p &= -p\mu_p\nabla(\psi q + kT \ln p) = -qp\mu_p\nabla\Phi_p \end{aligned} \right\} \quad (2.4)$$

where k is Boltzmann's constant, T is the lattice temperature (assumed constant), ψ is the electrostatic potential, Φ_n and Φ_p are the “electrochemical quasi-Fermi potentials” for electrons and holes. These definitions give

$$n = n_i \exp[(\psi - \Phi_n)/V_{th}] \quad \text{and} \quad p = n_i \exp[(-\psi + \Phi_p)/V_{th}]. \quad (2.5)$$

where $V_{th} = kT/q$ is called the thermal voltage. Here n_i is a constant called the intrinsic carrier density, and it represents the density of both holes and electrons in undoped silicon.

Gauss' equation for charge conservation and the conservation equations for holes and electrons can now be written

$$\left. \begin{aligned} \varepsilon \nabla \cdot \mathbf{E} &= -\varepsilon \nabla^2 \psi = \rho = q(p - n + N) \\ \frac{\partial n}{\partial t} - \frac{1}{q} \nabla \cdot \mathbf{J}_n &= G_n - U_n \\ \frac{\partial p}{\partial t} + \frac{1}{q} \nabla \cdot \mathbf{J}_p &= G_p - U_p \end{aligned} \right\} \quad (2.6)$$

where ε is the material dielectric constant, and $N = N_D - N_A$ is the static doping, comprising donors and acceptors. G_n, G_p are the electron and hole generation rates, and U_n, U_p are the electron and hole recombination rates. See Sze [S81] for expressions specifying the generation and recombination terms.

Equations (2.6), together with (2.4, 2.5), constitute three non-linear partial differential equations for the potentials ψ , Φ_n and Φ_p , in the most general context. This is the standard drift-diffusion model which has been the basis for most of the technical development of the semiconductor industry [S81, MRS 90].

In the application to current flow in an n -channel MOSFET, the holes are considered to be in thermal equilibrium, implying that Φ_p is constant, taken to be zero. Also the generation/recombination terms are omitted and only the case of time-independent currents is considered. For SPICE application this steady state approximation is good for circuits operating at frequencies less than 100MHz. For high frequency circuit applications SPICE steady state solutions are corrected by engineering approximations to include high frequency effects.

2.2 The Density Gradient Model for the Quantum Effect. The model employed in this paper is referred to in the semi-conductor literature as the DG model. This appellation derives from continuum mechanics (see [AT87], [AI89]): extensions from kinetic theory to the basic laws for a continuum which assume that the internal energy is a function of density give that the energy depends also on the spatial gradient of density. In the semiconductor context a similar extension to the DD model to include a quantum term may be obtained directly from the Schrödinger equation.

The classical quasi-Fermi potential in (2.5b), whose gradient is proportional to the force field extant in the continuum is, in the DG quantum extension, replaced by

$$\begin{aligned} \Phi_p &= \psi + V_{th} \ln(p/n_i) + \Phi_{qp} \\ \Phi_n &= \psi - V_{th} \ln(n/n_i) + \Phi_{qn} \end{aligned} \quad (2.7)$$

where

$$\begin{aligned}\Phi_{qp} &= 2b_n(\nabla^2\sqrt{p})/\sqrt{p}, \quad b_n = \hbar^2/12m^*q \\ \Phi_{qn} &= 2b_n(\nabla^2\sqrt{n})/\sqrt{n}, \quad b_n = \hbar^2/12m^*q\end{aligned}$$

where \hbar is Planck's constant. The factor m^* represents the hole effective mass normal to the interface (the holes are not quantized transverse to the interface). This factor is usually used as a fitting parameter, see [AYLDV07].

2.3 The Boundary Value Problem. Equations (2.6), amended by the assumptions discussed at the end of Section 2.1, together with equations (2.4b), (2.7), relating Φ_p with p and Φ_n with n comprise the field equations in the silicon $0 < x_1 < \infty$, $0 < x_2 < L$, where L is the channel length. No variation with x_3 is considered. The silicon region is adjoined by the oxide, $-t_{ox} < x_1 < 0$, in which no charges are assumed to reside, giving $\nabla \cdot \mathbf{E} = 0$ there.

The following boundary conditions on ψ and Φ_p are standard (see [WOC90]) :

$$\begin{aligned}\psi|_{x_1=-t_{ox}} &= V_{GS} - V_{FB}, \quad \psi|_{x_1 \rightarrow \infty} = -V_{th} \ln(N_A/n_i) \\ (\psi, \Phi_p)|_{x_2=0} &= (V_{th} \ln(N_A/n_i), 0) \\ (\psi, \Phi_p)|_{x_2=L} &= (V_{DS} + V_{th} \ln(N_A/n_i), V_{DS})\end{aligned}\tag{2.8}$$

In the above V_{GS} , V_{FB} and V_{DS} are gate, flat-band and drain voltages, N_D and N_A are the source/drain and silicon doping levels, respectively, and t_{ox} is the oxide thickness. No current leaves the device across $x_1 = 0$ or at $x_1 = \infty$. Since the PDE system described above contains two more derivatives than the classical system, two extra boundary conditions must be prescribed. These are taken to be

$$p = 0 \text{ at } x_1 = 0 \text{ and } p \rightarrow n_i^2/N_A \text{ as } x_1 \rightarrow \infty\tag{2.9}$$

Condition (2.15a) is consistent with quantum continuity of hole density and the assumption of zero density in the oxide. Condition (2.9b) is adopted on the basis that, though quantum effects alter the solution close to the gate interface region, the solution in the silicon bulk returns to its classical values. It is noted that in simulations using the full Schrödinger wave function Ψ the boundary conditions are taken to be $\Psi = 0$ at $x_1 = 0$ and at $x_1 = \infty$. The first condition is equivalent to (2.9a) and the second is not dissimilar to (2.9b) since n_i^2/N_A is many orders of magnitude smaller than the hole densities in the accumulation region.

2.4 Scaled Variables. In order to facilitate the use of the MOSFET $I-V$ results obtained in [CAM01] for the non-quantum case, we employ the

scaling used there; it was introduced by Ward in [WOC90]. The scaling is

$$\begin{aligned} (x_1, t_{ox}) &= (x, t)L_D\sqrt{2(\ln \lambda)/\lambda}, \quad x_2 = yL, \quad (\psi, \Phi_p) = (w, \varphi)V_{th} \ln \lambda \\ V_{DS} &= V_{ds}V_{th}, \quad V_{GS} - V_{FB} = V_{gs}V_{th} \ln \lambda \end{aligned} \quad (2.10)$$

where $L_D = \left(\frac{kT\epsilon_{si}}{2n_iq^2}\right)^{1/2}$ is called the intrinsic Debye length, and $\lambda = N_A/n_i$. This definition of L_D , in accord with current practice in the semi-conductor literature, has a $1/\sqrt{2}$ factor not present in previous publications [WOC90, W92, CAM01, AC03, AC04]. In the above, N_A is the substrate doping, typically of order $10^{15} - 10^{17} \text{ cm}^{-3}$, giving $\lambda \sim 10^5 - 10^7$. The scaling in (2.10) yields $O(1)$ changes in the scaled potential over the $O(1)$ changes in x that represent the depletion depth.

The reduction to ordinary differential equations is afforded by the quasi-one-dimensional approximation, which is valid for large aspect-ratio devices ($L \gg$ depletion depth), see [WOC90, CAM01].

With this scaling, the quasi-1-D drift-diffusion equations reduce to

$$\left. \begin{aligned} w_{xx} &= 0 & \text{in } -t < x < 0 \\ w_{xx} &= (n-p)/N_A + 1 & \text{in } x > 0 \end{aligned} \right\} \quad (2.11)$$

neglect p in accumulation

The quantum revisions to n and p , equation (2.8), become

$$\begin{aligned} 1 - w &= \frac{1}{\ln \lambda} \ln \left(\frac{p}{n_i} \right) - \frac{\lambda\beta^2}{(\ln \lambda)^2} \frac{1}{\sqrt{p}} \frac{d^2 \sqrt{p}}{dx^2} \\ w - \varphi &= \frac{1}{\ln \lambda} \ln \left(\frac{n}{n_i} \right) - \frac{\lambda\beta^2}{(\ln \lambda)^2} \frac{1}{\sqrt{n}} \frac{d^2 \sqrt{n}}{dx^2} \end{aligned} \quad (2.12)$$

where $\beta^2 = 2b_n/V_{th}L_D^2$.

Equation (2.11a) gives a linear potential in the oxide so that the continuity of electrostatic potential and displacement at the silicon/silicon dioxide interface yield boundary conditions there for equations (2.9b)-(2.11) as

$$n = 0 \quad p = 0 \quad \text{and} \quad \frac{\partial w}{\partial x} = c(w - V_{gs}) \quad \text{at} \quad x = 0 \quad (2.20)$$

$$\text{where } c = \sqrt{2 \ln \lambda / \lambda \epsilon_{ox}} L_D / \epsilon_{si} t_{ox}$$

and $\epsilon_{si}, \epsilon_{ox}$ are the dielectric constants of silicon and silicon dioxide.

Boundary conditions in the silicon bulk are

$$p \rightarrow N_A, \quad \text{and} \quad w \rightarrow 0 \quad \text{as} \quad x \rightarrow \infty, \quad (2.21)$$

In (2.12) the factor $\beta^2\lambda/(\ln \lambda)^2$ is $O(10^{-4})$ for $\lambda = 10^7$. This indicates that the quantum correction term is significant in a layer much smaller

than the depletion length and a fraction of the length scale of the accumulation layer. Outside this narrow quantum layer this term has the effect of shifting the classical solution away from the interface. Numerical solutions confirm this behavior showing that the QM effect on the electron density is substantial in a narrow layer close to the oxide interface, reducing it from high values to zero at the interface. (See Figure 1). The hole density is zero at the oxide interface with the accumulation charge peak at 5\AA to 15\AA . The solution of (2.12) in this narrow layer is called the inner solution.

3. Solution by Matched Asymptotic Expansions

3.1 Introduction. In the MAE technique, [B099, KC96], approximate solutions to the differential equations, valid in adjacent but overlapping regions, are blended together by suitably matching integration constants, resulting in a composite solution valid over the whole region of interest. Explicit solutions for the classical solution to equations (2.9)-(2.12) were developed in [CAM01], based on the MAE formulation presented in [W0C90, W92].

3.2 Inner and Outer Expansions. We now take up the solutions to equations (2.11), (2.12) based on formal expansions in $\varepsilon \ll 1$, where ε is defined by

$$\varepsilon^2 = \lambda\beta^2/2 \ln \lambda \quad (3.1)$$

In this section only the quantum effect on the accumulation layer is investigated: the electrons (n) in (2.11) are neglected, since $w < 0$ in the quantum/accumulation region. The system (2.11)-(2.12) is in conventional MAE format, with the small parameter multiplying the highest derivative term, indicating that the quantum layer thickness is much smaller than the reference length. For $\lambda = 10^5, 10^6, 10^7$ the reference length is 354nm, 123nm, 42nm, respectively, and the accumulation layer ($O(1/\ln \lambda)$ of the reference length) is then 30nm, 9nm, 2.6nm for these cases. We also assume that the quantum layer thickness (1-3nm in numerical solutions) is smaller than the accumulation layer depth. This assumption looks tenuous at the higher doping levels for which the accumulation layer thins.

Quantum Layer : Inner Expansion. For this expansion we prefer to use w and

$$T = \sqrt{p/n_i} \quad \text{or} \quad Y = \ln(p/n_i)/\ln \lambda \quad (3.2)$$

as dependent variables. The latter are equivalent and are used interchangeably, depending on which gives advantages in ease of solution. For the quantum inner layer the length scale is $O(\varepsilon)$ and the inner variable X given by

$$X = x/\varepsilon \quad (3.3)$$

is appropriate. With (3.2)-(3.3), equations (2.9) and (2.11) in terms of X become

$$\frac{d^2 w}{dX^2} = \varepsilon^2 \{1 - \exp[(Y - 1) \ln \lambda]\}, \quad (3.4)$$

$$\text{and } T^{-1} \frac{d^2 T}{dX^2} = \ln T + \ln \lambda (w - 1)/2 \quad (3.5)$$

$$\text{or } \frac{d^2 Y}{dX^2} + \frac{1}{2} \ln \lambda \left(\frac{dY}{dX} \right)^2 + 1 - w - Y = 0. \quad (3.6)$$

The expansions for w , T , Y are written as

$$(w, T, Y) = (W_0, T_0, Y_0) + \varepsilon (W_1, T_1, Y_1) + \varepsilon^2 (W_2, T_2, Y_2) + \dots \quad (3.7)$$

Substituting these into (3.4), (3.5) gives

$$W_0'' = 0 \rightarrow W_0 = W_{0s} + s_0 X, \quad (3.8)$$

$$W_1'' = 0 \rightarrow W_1 = W_{1s} + s_1 X, \quad (3.9)$$

$$W_2'' = 1 - T_0^2/\lambda, \quad (3.10)$$

$$T_0'' - T_0 \ln T_0 - \ln \lambda (W_0 - 1) T_0/2 = 0, \quad (3.11)$$

$$Y_1'' + \ln \lambda Y_0' Y_1' - W_1 - Y_1 = 0. \quad (3.12)$$

together with the relationships

$$T_0 = \exp(\ln \lambda Y_0/2) \quad \text{and} \quad T_1 = \ln \lambda T_0 Y_1/2 \quad (3.13)$$

etc. The boundary condition (2.20), and (3.8), (3.9), yield

$$\begin{aligned} \left. \frac{\partial W_0}{\partial X} \right|_{X=0} &= s_0 = 0, \\ \left. \frac{\partial W_1}{\partial X} \right|_{X=0} &= s_1 = c(W_{0s} - V_{gs}), \\ \left. \frac{\partial W_2}{\partial X} \right|_{X=0} &= cW_{1s}, \end{aligned} \quad (3.14)$$

Outer Expansion. Here the quantum term is considered to be a small perturbation of the system (2.11), and the outer expansion reads

$$\begin{aligned} w &= w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + \dots \\ \sqrt{p/n_i} &= \tau_0 + \varepsilon \tau_1 + \varepsilon^2 \tau_2 + \dots \end{aligned} \quad (3.15)$$

The first terms satisfy

$$\frac{d^2 w_0}{dx^2} = 1 - \frac{1}{\lambda} \tau_0^2, \quad (w_0 - 1) \ln \lambda = -2 \ln \tau_0. \quad (3.17)$$

The second terms satisfy

$$\frac{d^2 w_1}{dx^2} = -\frac{2}{\lambda} \tau_0 \tau_1, \quad w_1 \lambda = -2 \tau_1 / \tau_0, \quad (3.18)$$

giving

$$\frac{d^2 w_1}{dx^2} = \frac{\ln \lambda}{\lambda} \tau_0^2 w_1 \quad (3.19)$$

The outer solutions for w and Y are identical to $0(\varepsilon)$, see (2.11).

3.30 Solutions and Matching For accumulation the first term in the outer expansion satisfies:

$$w_0'' = 1 - e^{-w_0 \ln \lambda} \quad (3.20)$$

This equation may be integrated directly, however this gives rise to a solution in inverse form (x in terms of w). This is difficult to use with the inner quantum solution, therefore a layer solution is organized consisting of a solution valid when the exponential term on the right hand side of 3.20 is dominant, and a transition solution. The former is valid in a region where $x \approx \frac{1}{\ln \lambda}$ and is obtained using the following scaling:

$$x^* = \frac{x}{\frac{1}{\ln \lambda}} = x \ln \lambda$$

and the expansion

$$w_0(x^*) = w_{00} + \frac{1}{(\ln \lambda)^2} w_{01} + \dots \quad (3.21)$$

where w_{00} , and w_{01} satisfy

$$\frac{dw_{00}}{dx^{*2}} = -\frac{1}{(\ln \lambda)^2} e^{-w_{00} \ln \lambda}$$

and

$$\frac{dw_{01}}{dx^{*2}} = 1 + \frac{1}{\ln \lambda} w_{01} e^{-w_{01} \ln \lambda}$$

The following solution for w_{00} is selected,

$$w_{00} = -\frac{1}{\ln \lambda} \ln(2\alpha^2 \ln \lambda) - \frac{2}{\ln \lambda} \ln(\sec(\alpha x^2 + \gamma)) \quad (3.22)$$

The boundary condition at $x = 0$ yields

$$w_{0s} = -\frac{1}{\ln \lambda} \ln(2\alpha^2 \ln \lambda) - \frac{2}{\ln \lambda} \ln(\sec(\gamma)) = -\frac{1}{\ln \lambda} \ln(2\alpha^2 \ln \lambda \sec^2 \gamma) \quad (3.23)$$

3.31 Transition Solution The solution (3.21) must be blended with the bulk solution, $w_0 = 0$. This is achieved through a transition solution, which is valid over a region, $x \approx \frac{1}{\sqrt{\ln \lambda}}$. The scaled variable \hat{x} is defined by $\hat{x} = x\sqrt{\ln \lambda}$. The transition solution is

$$w_0 = -\frac{1}{\ln \lambda} u(\hat{x}) \quad (3.24)$$

so that (3.23) integrates to yield,

$$-\sqrt{2}\hat{x} = \int_{u_0}^u (e^y - y - 1)^{\frac{1}{2}} dy \quad (3.25)$$

where u_0 is an integration constant to be determined by matching with the accumulation layer solution (3.22). A second integration constant has been chosen so that (3.25) has the property that $u \rightarrow 0$ gives $\hat{x} \rightarrow 0$, and hence this solution blends with the bulk solution.

3.41 Matching Solutions The constant u_0 is determined by matching with the solution for w_{00} given in (3.22). Matching the two solutions (3.22) and (3.25) is determined through a matching region $\eta(\lambda)$ where,

$$\frac{1}{\ln\lambda} \ll \eta \ll \frac{1}{\sqrt{\ln\lambda}}$$

and the variable x_η is given by

$$x_\eta = \frac{x}{\eta}$$

In this matching of the solutions, the method for matching in [W92] was followed closely yielding,

$$w_{00} = -\frac{1}{\ln\lambda} \ln(2\alpha^2 \ln\lambda \sec^2 \gamma) - \frac{2}{\ln\lambda} \tan\gamma (\alpha \ln\lambda) \eta x_\eta + \dots \quad (3.26)$$

and

$$u = u_0 - (\sqrt{2\ln\lambda}) \eta x_\eta (e^{u_0} - u_0 - 1)^{\frac{1}{2}} + \frac{1}{2} (\ln\lambda) \eta^2 x_\eta^2 (e^{u_0} - 1) + \dots \quad (3.27)$$

Finally matching these solutions gives the equations as follows:

$$w_{0s} = -\frac{u_0}{\ln\lambda} \quad (3.28)$$

and

$$2\alpha \tan\gamma = -\sqrt{\frac{2}{\ln\lambda}} (e^{u_0} - u_0 - 1)^{\frac{1}{2}} \quad (3.29)$$

Equations (3.23), (3.29), and (3.44) give us α , γ and u_0 in terms of w_{0s} .

4. The First Integral

Next is to derive a first integral from the original equations. The preceding work was necessary in order to have explicit formula for terms in the equations which we will now derive.

4.11 **Inversion** Here the steps are repeated in the work done by the Clinic in 2005-2006, [AFY06]. The focus will be on the inversion region after which the analog result will be given for the Accumulation region. Just as a reminder the original equations we are interested in are

$$\begin{aligned} w'' &= \frac{n-p}{N_A} + 1 \\ w - \phi &= \frac{1}{\ln \lambda} \ln \frac{n}{n_i} - \frac{\beta^2 \lambda}{(\ln \lambda)^2} \frac{1}{\sqrt{n}} \frac{d^2 \sqrt{n}}{dx^2} \end{aligned}$$

along with the boundary condition that

$$w'(0) = w'_s = r(w_s - v), \quad n(0) = 0$$

where $w_s = w(0)$. A substitution $a^2 = n$ allows the derivation of the following relationships

$$w'' = \frac{a^2 - p}{N_A} + 1 \quad (4.1)$$

$$w - \phi = \frac{1}{\ln \lambda} \ln \frac{a^2}{n_i} - \frac{\beta^2 \lambda}{(\ln \lambda)^2} \frac{a''}{a} \quad (4.2)$$

The next step is to multiply equation (4.1) by w' , write p explicitly, and move the terms around

$$a^2 w' = N_A (w' w'' - w') + w' n_i e^{(w-\phi) \ln \lambda}. \quad (4.3)$$

Consider equation (4.2) when it has been multiplied by aa' , and derive that

$$aa' w - aa' \phi = \frac{aa'}{2 \ln \lambda} \ln \frac{a}{\sqrt{n_i}} - \frac{\beta^2 \lambda}{(\ln \lambda)^2} a'' a' \quad (4.4)$$

Note that $a'' a' = \left(\frac{(a')^2}{2}\right)'$, and similarly $aa' = \left(\frac{(a^2)}{2}\right)'$, and rewrite the above equation as

$$aa' w - \phi \left(\frac{a^2}{2}\right)' = -\frac{\beta^2 \lambda}{(\ln \lambda)^2} \left(\frac{(a')^2}{2}\right)' + \frac{1}{2 \ln \lambda} \left(a^2 \left(2 \ln \frac{a}{\sqrt{n_i}} - 1\right)\right)'$$

Explicitly derivating the last term in the above equation shows that in fact we get back the original equation. Let us consider

$$\frac{1}{2 \ln \lambda} \left(a^2 \left(\ln \frac{a^2}{n_i} - 1\right)\right)'$$

and calculate the derivate. The derivative follows

$$\begin{aligned}
& \frac{1}{2 \ln \lambda} \left(2aa' \left(\ln \frac{a^2}{n_i} - 1 \right) + a^2 \left(\frac{2a'}{a} \right) \right) \\
&= \frac{aa'}{\ln \lambda} \ln \frac{a^2}{n_i} + \frac{1}{2 \ln \lambda} (-2aa + 2aa') \\
&= \frac{aa'}{2 \ln \lambda} \ln \frac{a}{\sqrt{n_i}}
\end{aligned}$$

and this is one of the terms in equation (4.4). Before finishing the first integral note the identity $(a^2 w)' = 2aa'w + a^2 w'$ by use of the Chain Rule. Multiplying equation (4.3) by $\frac{1}{2}$ and adding the result to equation (4.4) yields

$$\begin{aligned}
\frac{a^2 w'}{2} + aa'w - \phi \left(\frac{a^2}{2} \right)' &= \frac{N_A}{2} (w'w'' - w') + \frac{1}{2} w' n_i e^{(w-\phi) \ln \lambda} \\
&\quad - \frac{\beta^2 \lambda}{(\ln \lambda)^2} \left(\left(\frac{a'}{2} \right)^2 \right)' + \frac{1}{2 \ln \lambda} \left(a^2 \left(2 \ln \frac{a}{\sqrt{n_i}} - 1 \right) \right)' .
\end{aligned}$$

Now all of the terms can be integrated once in the above equation after the first two terms are combined as $\left(\frac{a^2 w}{2} \right)'$. Hence the first integral in inversion is obtained as

$$\begin{aligned}
& \frac{a^2 w}{2} - \frac{N_A}{2} \left(\frac{(w')^2}{2} - w \right) + \frac{n_i}{2 \ln \lambda} e^{-w \ln \lambda} - \frac{a^2 \phi}{2} \\
&= \frac{a^2}{\ln \lambda} \ln \frac{a}{\sqrt{n_i}} - \frac{a^2}{2 \ln \lambda} - \frac{\beta^2 \lambda}{(\ln \lambda)^2} \frac{(a')^2}{2} + \frac{I_{ci}}{2}
\end{aligned}$$

where I_{ci} is the integration constant. A consideration of the boundary conditions allows a simplification to

$$w'_s = -\sqrt{2} \left(w_s + \frac{e^{-w_s \ln \lambda}}{\lambda \ln \lambda} + \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)^2} - \frac{I_{ci}}{N_A} \right)^{\frac{1}{2}} . \quad (4.5)$$

4.12 Accumulation

Using the same methods in the previous section a derivation of the first integral for the Accumulation Region is straightforward. The difference here is that (4.2) is replaced by

$$w - \phi = K \frac{1}{\sqrt{p}} \frac{d\sqrt{p}}{dx^2} - \frac{1}{\ln \lambda} \ln \frac{p}{n_i} .$$

Putting $\beta^2 = p$ and following the development in Section [4.11] gives

$$(w'_s)^2 = 2w_s + \frac{2n_i e^{(w_s - \phi) \ln \lambda}}{N_A \ln \lambda} + 2K(b'(0))^2 + \frac{4I_{ca}}{N_A} \quad (4.6)$$

where K is a constant related to the quantum correction.

4.2 Lambert Function

This section will concern itself with finding explicit formulas for w_s in terms of w'_s using the Lambert function.

4.21 **Inversion** Given the first integral, the approach is to find an analytic solution for w_s . Introducing the Lambert Omega Function is needed which is defined as the inverse of $f(x) = xe^x$. The Lambert Function is often written as $x = We^W$. This function is multivalued and so a branch must be chosen. For presentation purposes $q = -w'_s$, and hence $q^2 = (w'_s)^2$. This substitution into equation (4.5) yields

$$\frac{q^2}{2} = w_s + \frac{e^{-w_s \ln \lambda}}{\lambda \ln \lambda} + \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)^2} - \frac{I_{ci}}{N_A}$$

which can again be rewritten as

$$-\ln \lambda \frac{q^2}{2} - \ln \lambda \frac{I_{ci}}{N_A} + w_s \ln \lambda + \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)} = -\frac{e^{-w_s \ln \lambda}}{\lambda}.$$

The next step is to multiply both sides of the above equation by e^{RHS} where RHS is the right hand side of the equation. The result is

$$RHS e^{RHS} = -\frac{1}{\lambda} e^{-\ln \lambda \frac{q^2}{2} - \ln \lambda \frac{I_{ci}}{N_A} + \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)}}.$$

Now the Lambert Function can be applied, simplified as LW,

$$\begin{aligned} & -\ln \lambda \frac{q^2}{2} - \ln \lambda \frac{I_{ci}}{N_A} + w_s \ln \lambda + \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)} \\ &= LW \left(-\frac{1}{\lambda} e^{-\ln \lambda \frac{q^2}{2} - \ln \lambda \frac{I_{ci}}{N_A} + \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)}} \right) \end{aligned}$$

resulting in a formula strictly in terms of w_s

$$w_s = \frac{q^2}{2} + \frac{I_{ci}}{N_A} - \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)^2} + \frac{1}{\ln \lambda} LW \left(-\frac{1}{\lambda} e^{-\ln \lambda \frac{q^2}{2} - \ln \lambda \frac{I_{ci}}{N_A} + \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)}} \right) \quad (4.6)$$

4.22 Accumulation

In accumulation the explicit formula for w_s follows from (4.6) using the same procedure as in Section [4.21]:

$$w_s = -\frac{2I_{ca}}{N_A} - \frac{K(b'(0))^2}{N_A} + \frac{q^2}{2} - \frac{1}{\ln \lambda} LW \left(\frac{n_i}{N_A \ln \lambda} e^{-\phi \ln \lambda - \frac{2I_{ca} \ln \lambda}{N_A} - \frac{K \ln \lambda (b'(0))^2}{N_A} + \frac{q^2 \ln \lambda}{2}} \right) \quad (4.7)$$

4.3 Estimating $a'(0)$

In order to use equation (4.6) an estimate of $a'(0)$ is required. Here is shown how this may be calculated using the results from [CUA07]. A

parallel development to find $b'(0)$ in equation (4.7) using the work done in Section [3], is the first task of the new semester.

Here for inversion, we use $T = \sqrt{n/n_i}$ or $Y = \ln(n/n_i)/\ln\lambda$ as dependent variables. From the definition, $a = \sqrt{n}$, so $a'(0) = \sqrt{n_i}T'(0)$.

$$\begin{aligned} T &= T_0 + \varepsilon T_1 + \dots \\ Y &= Y_0 + \varepsilon Y_1 + \dots \end{aligned}$$

Because T and Y are equivalent and interchangeable, based on their relationship $T^2 = \lambda^Y$, the following equation is aquired

$$T_1 = \frac{1}{2}\ln\lambda T_0 Y_1 \quad (4.7)$$

In [CUA01], the equation for the inner solution of inversion would lead to

$$S_0'' = S_0 \ln S_0 \quad \text{where} \quad S_0 = T_0/\tau_{0s} \quad (4.8)$$

This has the solution

$$X = \int_0^{S_0} (s^2 \ln s + (1 - s^2)/2)^{-1/2} ds. \quad (4.9)$$

Since $S_0(0) = 0$, it follows that

$$\begin{aligned} \frac{dX}{dS_0} \Big|_{X=0} &= (S_0^2 \ln S_0 + \frac{1-S_0^2}{2})^{-1/2} \\ &= (\frac{1}{2})^{-1/2} = \sqrt{2}. \end{aligned} \quad (4.10)$$

Using the chain rule

$$\frac{dT_0}{dX} \Big|_{X=0} = \frac{dT_0}{dS_0} \Big|_{X=0} \cdot \frac{dS_0}{dX} \Big|_{X=0} = \frac{1}{\sqrt{2}} \tau_{0s}. \quad (4.11)$$

and so the first part is done.

From (4.7) the derivative of T_1 is

$$\frac{dT_1}{dX} = \frac{1}{2}\ln\lambda \left(\frac{dT_0}{dX} Y_1 + T_0 \frac{dY_1}{dX} \right) \quad (4.12)$$

Also in [CUA02], the equation for the inner solution of inversion would become that

$$Y_1'' + 2(S_0'/S_0)Y_1' - Y_1 = -W_{1s} - s_1 X \quad (4.13)$$

This has the solution

$$\begin{aligned} Y_1 &= \frac{1}{3}e^{-X}(1 - e^X)^{-1} \{ E_1(1 + 3e^X) + E_2(1 + e^X)^3 - W_{1s}(2 + 3e^X + 3e^{2X}) \\ &\quad + s_1(2e^X + 2e^{2X} + 3Xe^X + 3Xe^{2X} + 2Xe^{3X} \\ &\quad - 2(1 + 3e^X + 3e^{2X} + e^{3X}) \ln(1 + e^X) \} \end{aligned} \quad (4.14)$$

Since the E_2 term is exponentially large at $X \gg 1$, $E_2 = 0$ and

$$E_1 = 2W_{1s} + s_1(1 - 4 \ln 2) \quad (4.15)$$

L'Hopital's Rule is now used

$$Y_1|_{X=0} \rightarrow W_{1s} + S_1(12 \ln 2 - 3) \quad (4.16)$$

To calculate $\frac{dY_1}{dX}|_{X=0}$, apply L'Hopital's Rule twice to see that

$$\frac{dY_1}{dX}|_{X=0} = 0 \quad (4.17)$$

Putting (4.11), (4.16) and (4.17) together and conclude that

$$\begin{aligned} a'(0) &= \sqrt{n_i} \frac{dT}{dX}|_{X=0} \\ &= \sqrt{n_i} \left[\frac{dT_0}{dX}|_{X=0} + \varepsilon \frac{dT_1}{dX}|_{X=0} \right] \\ &= \sqrt{n_i} \left\{ \frac{1}{\sqrt{2}} \tau_{0s} + \varepsilon \left[\frac{1}{2} \ln \lambda \left(\frac{1}{\sqrt{2}} \tau_{0s} (W_{1s} + S_1(12 \ln 2 - 3)) \right) \right] \right\} \end{aligned}$$

an explicit expression for what we believe to be a reasonable estimate for $a'(0)$.

5. Capacitance

Now the focus turns to the capacitance from the gate to the base. The capacitance is given by $c = -\frac{dw'_s}{dv} = \frac{dq}{dv}$. From the boundary condition we also know that $v = w_s + \frac{q}{r}$ and so it makes it easier to calculate $c^{-1} = \frac{dq}{dv} = \frac{dw_s}{dq} + \frac{1}{r}$. Now we can invert this and get that

$$c = \frac{r}{r \frac{dw'_s}{dq} + 1}$$

and using the results from sections [4.21] and [4.22] we can calculate $\frac{dw_s}{dq}$ to give c in the inversion and accumulation regimes, respectively. We use that fact that $\frac{d}{dz} LW(z) = \frac{LW}{z(1+LW)}$ for $z \neq \frac{-1}{e}$ and $z \neq 0$. For inversion

$$w'_s(q) = q + \frac{1}{\ln \lambda} \left(\frac{LW(z)}{1 + LW(z)} \right) q \ln \lambda$$

and for accumulation we have that

$$w'_s(q) = q - \frac{1}{\ln \lambda} \left(\frac{LW(y)}{1 + LW(y)} \right) (-q \ln \lambda)$$

for

$$z = -\frac{1}{\lambda} e^{-\ln \lambda \frac{q^2}{2} - \ln \lambda \frac{I_{ci}}{N_A} + \frac{(a'(0))^2 \beta^2 \lambda}{N_A (\ln \lambda)}}$$

and

$$y = \frac{n_i}{N_A \ln \lambda} e^{-\phi \ln \lambda - \frac{2I_{cq} \ln \lambda}{N_A} - \frac{K \ln \lambda (b'(0))^2}{N_A} + \frac{q^2 \ln \lambda}{2}}.$$

6. Continuing Work.

All of the necessary ingredients are now available in order to begin an analysis of the accuracy of these results against data. An analytic expression for the capacitance has been obtained in terms of a parameter q which is ultimately a function of the voltage. This is a transcendental equation and our attempts to solve it numerically will consist of applying Newton's Method. This will be facilitated by the fact that the solution is very similar to this solution to the classical model under the drift diffusion equations. An attempt to blend the regions will be made and we expect to be able to get positive results following the methods used for classical PMOS modeling as done by Cumberbatch and Morris [CM01].

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