THEORETICAL BACKGROUND

1. Drift-diffusion approximation for basic semiconductor equations (1-D)

Basic semiconductor equations (BSE) are continuity equations for carrier concentrations, equations for current density and Poisson equation for electrostatic potential. Equations for current density are not very interesting so we skip them here as well as normalization procedure.

Continuity equation for electrons:

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial x}\left[\mu_n\left(n\frac{\partial \varphi}{\partial x} - \frac{\partial n}{\partial x}\right)\right] + R\ , \tag{1}$$

where n – electron concentration;
t – time;
x – coordinate;
μ_n – electron mobility;
φ – electrostatic potential;
R – generation-recombination term.

Continuity equation for holes:

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left[\mu_n\left(p\frac{\partial \varphi}{\partial x} + \frac{\partial p}{\partial x}\right)\right] + R\ . \tag{2}$$

where p – hole concentration;
t – time;
x – coordinate;
μ_p – hole mobility;
φ – electrostatic potential;
R – generation-recombination term.

Poisson equation:

$$\frac{\partial^2 \varphi}{\partial x^2} = n - p - N_D + N_A\ , \tag{3}$$

where φ – electrostatic potential;
x – coordinate;
p – hole concentration;
n – electron concentration;
N_D – donor concentration;
N_A – acceptor concentration.

2. Transition to the quasi-Fermi exponential basis

Quasi-Fermi basis:

$$\begin{aligned} \varphi_n &= \ln(n) - \varphi\ ; \\ \varphi_p &= \ln(p) + \varphi\ , \end{aligned} \tag{4}$$

where φ – electrostatic potential;
φ_n – quasi-Fermi level for electrons;

φ_p – quasi-Fermi level for holes;
p – hole concentration;
n – electron concentration.

Concentrations:

$$n = \exp(\varphi_n + \varphi) \ ; \qquad p = \exp(\varphi_p - \varphi) \ , \tag{5}$$

where φ – electrostatic potential;
φ_n – quasi-Fermi level for electrons;
φ_p – quasi-Fermi level for holes;
p – hole concentration;
n – electron concentration.

Quasi-Fermi exponential basis:

$$\Phi_n = \exp(\varphi_n) \ ; \qquad \Phi_p = \exp(\varphi_p) \ , \tag{6}$$

where Φ_n – quasi-Fermi exponent for electrons;
Φ_p – quasi-Fermi exponent for holes;
φ_n – quasi-Fermi level for electrons;
φ_p – quasi-Fermi level for holes.

If we substitute the expressions (5) in equations (1, 2, 3) then after simplification we obtain:

$$\begin{gathered}
\frac{\partial}{\partial t}[\exp(\varphi_n + \varphi)] = \frac{\partial}{\partial x}\left[\mu_n \exp(\varphi_n + \varphi)\frac{\partial \varphi_n}{\partial x}\right] + R \ ; \\
\frac{\partial}{\partial t}[\exp(\varphi_p - \varphi)] = \frac{\partial}{\partial x}\left[\mu_p \exp(\varphi_p - \varphi)\frac{\partial \varphi_p}{\partial x}\right] + R \ ; \\
\frac{\partial^2 \varphi}{\partial x^2} = \exp(\varphi_n + \varphi) - \exp(\varphi_p - \varphi) - N_D + N_A \ .
\end{gathered} \tag{7}$$

Thus we have a system of basic semiconductor equations in the basis of quasi-Fermi levels and electrostatic potential. Now we need to transit obtained system to the quasi-Fermi exponential basis.

Considering expressions (6) and after some simplification (It is simple but cumbersome, so it's best to do it yourself on paper) equations (7) take the form:

$$\begin{gathered}
\frac{\partial}{\partial t}[\Phi_n \exp(\varphi)] = \frac{\partial}{\partial x}\left[\mu_n \exp(\varphi)\frac{\partial \Phi_n}{\partial x}\right] + R \ ; \\
\frac{\partial}{\partial t}[\Phi_p \exp(-\varphi)] = \frac{\partial}{\partial x}\left[\mu_p \exp(-\varphi)\frac{\partial \Phi_p}{\partial x}\right] + R \ ; \\
\frac{\partial^2 \varphi}{\partial x^2} = \Phi_n \exp(\varphi) - \Phi_p \exp(-\varphi) - N_D + N_A \ .
\end{gathered} \tag{8}$$

This basis provides a good convergence for intense injection, so there is no reason to use something else. I think even for educational tasks that one is good enough.

For convenience equations (8) can be written:

$$\frac{\partial}{\partial t}[\Phi_n e^{\varphi}]=\frac{\partial}{\partial x}\left[\mu_n e^{\varphi}\frac{\partial \Phi_n}{\partial x}\right]+R\ ;$$
$$\frac{\partial}{\partial t}[\Phi_p e^{-\varphi}]=\frac{\partial}{\partial x}\left[\mu_p e^{-\varphi}\frac{\partial \Phi_p}{\partial x}\right]+R\ ; \qquad (8^*)$$
$$\frac{\partial^2 \varphi}{\partial x^2}=\Phi_n e^{\varphi}-\Phi_p e^{-\varphi}-N_D+N_A\ .$$

For stationary problem we should take:

$$\frac{\partial}{\partial t}[\Phi_n e^{\varphi}]=0\ ;$$
$$\frac{\partial}{\partial t}[\Phi_p e^{-\varphi}]=0\ ; \qquad (9)$$
$$R=0\ .$$

After all Simplified BSE takes form:

$$\frac{\partial}{\partial x}\left[\mu_n e^{\varphi}\frac{\partial \Phi_n}{\partial x}\right]=0\ ;$$
$$\frac{\partial}{\partial x}\left[\mu_p e^{-\varphi}\frac{\partial \Phi_p}{\partial x}\right]=0\ ; \qquad (10)$$
$$\frac{\partial^2 \varphi}{\partial x^2}=\Phi_n e^{\varphi}-\Phi_p e^{-\varphi}-N\ ,$$

where Φ_n – quasi-Fermi exponent for electrons;
Φ_p – quasi-Fermi exponent for holes;
φ – electrostatic potential;
N – effective impurity concentration $N = N_D - N_A$.

This is actually the desired system. Now we need to set correct boundary conditions. Setting the correct boundary conditions is the main difficulty in solving the system, except for the numerical implementation nuances.

3. Boundary conditions

It is able to obtain boundary conditions for «concentration» basis:

$$n=\frac{N}{2}+\sqrt{\left(\frac{N}{2}\right)^2+1}\ ,\quad p=-\frac{N}{2}+\sqrt{\left(\frac{N}{2}\right)^2+1}\ ;$$
$$\varphi=\ln\left(\frac{N}{2}+\sqrt{\left(\frac{N}{2}\right)^2+1}\right)+U\ ,\quad \varphi=-\ln\left(-\frac{N}{2}+\sqrt{\left(\frac{N}{2}\right)^2+1}\right)+U\ , \qquad (11)$$

where U – bias voltage;
p – hole concentration;

n – electron concentration;
φ – electrostatic potential;
N – effective impurity concentration $N = N_D - N_A$.

Considering (5, 6, 11) one can obtain:

$$\Phi_n = \left(\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + 1}\right) \cdot e^{-\varphi} \; ;$$
$$\Phi_p = \left(-\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + 1}\right) \cdot e^{\varphi} \; . \tag{12}$$

After substitution (11) and simplification expressions (12) take form:

$$\Phi_n = e^{-U} \; ;$$
$$\Phi_p = e^{U} \; . \tag{13}$$

Full set of boundary conditions is:

$$\Phi_n = e^{-U} \; ;$$
$$\Phi_p = e^{U} \; ; \tag{13*}$$
$$\varphi = \ln\left(\frac{N}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + 1}\right) + U \; .$$