The low thermal conductivity of gallium arsenide compared to silicon results in self-heating effects in GaAs MESFETs that limit the electrical performance of such devices for high power applications. To date, analytical thermal models of self heating in GaAs MESFETs are based on the assumption of a uniformly heated channel. This thesis presents a two dimensional analysis of the electro-thermal effect of this device based on the two dimensional power density distribution in the channel under various bias conditions. The numerical simulation is performed using the finite difference technique. The results of the simulation of an isothermal MESFET without heat effects is compared with various one dimensional analytical models in the literature. Electro-thermal effects into the two-dimensional isothermal MESFET model allowed close examination of the temperature profile within the MESFET. The large gradient in power distribution results in a localized heat source within the channel which increases the overall channel temperature, which shows that the assumption of a uniformly heated channel is erroneous, and may lead to an underestimation of the maximum channel temperature.
A Two Dimensional Numerical Simulation of A Non–isothermal GaAs MESFET

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Typed by Angela A. Lin for Angela A. Lin
To my father and mother for their love and sacrifices.
To my grandmother for her example of faith and thanksgiving.

"Those who wait for the Lord will gain new strength;
They will mount up with wings like eagles,
They will run and not get tired,
They will walk and not become weary."

Isaiah 40:31
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A considerable volume of literature to date has emphasized the electrical differences between gallium arsenide (GaAs) and silicon (Si) for high speed integrated circuit technology. However, relatively little has been said about the differences in the thermal properties between the two types of materials. In the past, electro-thermal effects in silicon devices have not been considered in device simulations and circuit designs unless the device dissipates high power. Thermal considerations have been treated independently from device modeling without introducing significant error because silicon has relatively high thermal conductivity such that most of the heat dissipation is through the device package and the heat sink. The thermal conductivity of GaAs is only about one-third that of silicon at room temperature. Due to the lower thermal conductivity, a considerable thermal drop occurs in the device die. A higher device channel temperature reduces the long term reliability of a GaAs devices [Roesch, 1981], and causes non-ideal electrical characteristics, such as negative output conductance in GaAs Metal-Semiconductor Field-Effect Transistors (MESFETs).

Thermal modeling of GaAs MESFETs has been studied by various groups. Before the 1980s, research on the thermal modeling of MESFETs has been based only on the concept of thermal resistance. By assuming the entire active channel is isothermal and has uniform heat generation, the thermal resistance model provides an average temperature difference between the device channel and the
heat sink. These models do not account for the electro-thermal relationship within the channel which produces localized peak temperature sources in the high field and high current density regions. Using only the basic thermal resistance concept without an accurate model of localized heat generation, one can underestimate the peak temperature within a device. The localized "hot spots" within the non-isothermal channel causes an overall channel temperature increase which magnifies the effects in the electrical behavior predicted by the simple analytical models. In order to obtain a more accurate power density map, one needs the current and electrical field distribution within the device of interest. Webb performed a thermal resistance study of GaAs MESFETs using three dimensional numerical simulation of the heat equation and a model for power dissipation within a non-isothermal channel [Webb, 1989]. This power distribution model, shown in Fig. 1.1, is calculated based on an educated guess of the current density and field distribution within the channel. Although this model does provide a closer approximation to a real MESFET than the isothermal channel analytical models, the fixed power distribution model within the channel does not accurately describe the device since the current flow as well as the electrical field change with both the drain and gate bias. A more accurate simulation requires a knowledge of the exact power generation at each point in the channel. A numerical simulation which solves the fundamental semiconductor equations and heat transport equation with minimal assumptions will provide a more accurate model of the operation of the device.

The application of numerical methods to solve the semiconductor device equations appeared as early as 1964 with the work of H. K. Gummel [Gummel, 1964]. He introduced the use of the sequential iteration method, known as Gummel's algorithm, to solve the drift-diffusion equations that describe the
electrical characteristics of bipolar transistors. Until 1969, the majority of simulations performed were one dimensional models, which are sufficient for simulating devices with a one dimensional current flow pattern, such as bipolar transistors and diodes. Simulation of two-dimensional effects was first used to study current spreading and base widening effects in bipolar transistors. Unlike bipolar transistors, FETs have a two dimensional current flow pattern that requires two-dimensional simulation. With various works performed over the years on Metal–Oxide–Silicon Field–Effect Transistors (MOSFETs), MESFETs and Modulation–Doped Field–Effect Transistors (MODFETs), the numerical techniques for solving two-dimensional problems are well established.

The application of numerical techniques to solve the combined electro–thermal effects was first used by Gaur and Navon in their study of the self–heating effects in npn power transistors [Gaur, 1976]. In addition to solving Poisson's equation and the drift–diffusion equations, the heat transport equation was incorporated into Gummel's loop. Similar techniques have since been used to simulate both the steady state and transient thermal response of bipolar power transistors [Alwin 1977, Chryssafis, 1979]. Ghione applied the same technique to solve two dimensional drift–diffusion and heat equations of GaAs MESFET to study the electro–thermal effects. The simulation results demonstrated the large variation in temperature distribution within the channel, and the localized peak temperature at the drain end of the gate. The electro–thermal effects are manifested in both the DC and AC performances, i.e. negative output conductance in the I–V characteristics, and the reduction in device gain, $|S_{21}|$, of the scattering parameters [Ghione, 1989]. Ghione's two dimensional simulation did not consider the thermal contributions of substrate depths and thermal conduction through the metal contacts, and the effects of thermal
radiation and convection, which are the reasons for back contact thinning, via holes and Flip−Chip design. Electro−thermal effects have also been studied using the Monte Carlo simulation. Moglestue simulated the pattern of heat development by taking into account of phonons absorbed and emitted by the charge carriers as they are being scattered by the lattice [Moglestue, 1981]. The limitation in using Monte Carlo simulation is the simulation time is of the order of tens of pico−seconds, while thermal effects usually reach steady state only after seconds of device operation. Thus, the simulation result provides a more accurate picture of the heat generation and cooling pattern in the device, but does not provide the steady state device temperature.

The purpose of this thesis is to develop a two−dimensional numerical model of a MESFET combining the drift−diffusion equations and the heat transport equation taking into account of substrate depth, and to study qualitatively the contribution of conduction through metal contacts, natural convection and radiation. The assumptions and approximations are minimized in order to provide a more accurate model of the device temperature profile and electro−thermal effects otherwise difficult or impossible to obtain with analytical models. Chapter Two discusses various one dimensional analytical models with and without thermal consideration. Chapter Three presents the implementation of the simulation program. The results of the two dimensional simulation are compared with the various analytical models in Chapter Four. Chapter Five concludes the thesis and discusses some of the limitations in the current work, and also gives suggestions for further work.
Figure 1.1 Webb's power generation distribution model [Webb, 1989].
Chapter Two

ONE DIMENSIONAL ANALYSIS

Isothermal Analytical Models

A MESFET consists of a conducting channel, two Ohmic contacts for the drain and the source, and a Schottky gate. Figure 2.1 shows the cross section of the MESFET under various bias conditions. One simple analytical model of a MESFET is based on the gradual channel approximation introduced by Shockley in the early 1950s. This one-dimensional analytical model assumes the region under the gate is completely depleted, the conducting channel is neutral, and the potential of the gate junction in the direction across the device is a slowly varying function of position along the gate. With these assumptions, the potential under the gate at a point along the channel may be expressed as a one dimensional function, and the current–voltage relation solved analytically. The current–voltage relationship of a MESFET with constant channel doping of \( N_D \) can be described by the equations \([\text{Sze, 1981}]\)

\[
I_{CH} = \frac{q\mu_0 N_D W A}{L_G} \left[ V_{DS} - \frac{2}{3} \left( \frac{(V_{DS} + V_{BI} - V_G)^{3/2} - (V_{BI} - V_G)^{3/2}}{V_{PO}^{1/2}} \right) \right],
\]

for \( V_{DS} < V_{DS^{SAT}} \), and

\[
I_{SAT} = \frac{q\mu_0 N_D W A}{L_G} \left[ \frac{1}{3} V_{PO} + \frac{2}{3} \frac{(V_{BI} - V_G)^{3/2}}{V_{PO}^{1/2}} - V_{BI} + V_G \right],
\]

for \( V_{DS} \geq V_{DS^{SAT}} \). The parameter \( V_{PO} \) is the pinch off voltage given by \( qN_DA^2/2\varepsilon_s \).

Silicon FETs typically saturate at pinch-off, where the depletion region at the drain side of the gate extends through the entire active channel. The built-in potential, \( V_{BI} \) is \( (E_C - E_F)/q + V_{BN} \), where \( V_{BN} \) is the Schottky barrier potential.

The surface states in the interfacial layer between the gate metal deposition and
the semiconductor surface determines the barrier height. For GaAs, $V_{BN}$ is about 0.8eV. $V_{DS}^{SAT}$ is the saturation voltage given by $V_{GS}+V_T$. And the threshold voltage is given by $V_T=V_{PO}+V_{BN}-V_{BI}$.

According to Shockley’s model, the electron velocity is proportional to the electric field by a constant which is the mobility. However, this linear relationship holds only at low electric field. At high field, velocity saturation occurs, and thus the device characteristics do not follow the assumptions used by Shockley’s model. The electron velocity of GaAs reaches peak around 3kV/cm compared to the 50kV/cm saturation field of silicon. Because of this, velocity saturation has a more significant effect on current saturation in GaAs MESFETs than in silicon FETs of the same gate length. For a short channel GaAs MESFET away from cut–off ($V_{GS}+V_T \gg 0$), the electric field $E_X$ reaches the critical saturation field before pinch–off occurs at the drain side of the gate. For this reason, the channel does not pinch–off completely but remains at $A-Ads(V_{DS})$, where $A$ is the channel depth and $Ads(V_{DS})$ is the depletion width at the drain end.

Referring to Fig. 2.1 which shows the changes in depletion region under various bias conditions, when $V_{DS}$ is small, the electric field in the conducting channel is less than the saturation field (point 1), and this corresponds to the linear region in the current voltage relationship, also known as the triode region. Velocity saturation starts at the drain edge of the gate (point 2). As $V_{DS}$ increases further, the high field region extends under the gate and the carriers in this region also reach the saturation velocity (point 3). The effective gate length $L_{EFF}$ is reduced by $L_S$, and the depletion depth decreases. This is known as channel length modulation, and the non–ideal characteristic is manifested in a finite output conductance. At even higher $V_{DS}$, the saturation region extends completely under the gate (point 4). Because current saturation in GaAs
MESFETs with short gate lengths is caused by electron velocity saturation and not channel pinch-off, Shockley's model does not provide an accurate estimate of the current-voltage relationship.

An alternative analytical expression which takes into account velocity saturation was proposed by Curtice [Curtice, 1980]. Electron velocity and electric field relationship may be approximated by an simplified piece-wise linear relationship to solve otherwise complicated drift and diffusion equations. Below the critical electric field, $F_S$, the velocity is proportional to the field. Saturation velocity, $v_s$, is maintained when the field reaches $F_S$ (see Fig. 2.2). To account for the earlier saturation in GaAs MESFETs due to the lower critical electric field and higher low field mobility, Curtice modified the FET model by adding the hyperbolic tangent function to model the current saturation mechanism. The resulting expression is

$$I_{DS0} = I_{DS0}^{SAT}(1 + \lambda V_{DS}) \tanh(\alpha V_{DS})$$

where $I_{DS0}^{SAT} = \beta \cdot (V_{GS} - V_T)^2$, and where $\lambda$ and $\alpha$ are empirical constants which account for the output conductance and saturation respectively. $\beta$ is the transconductance parameter given by [Shur, 1987]

$$\beta = \frac{2\varepsilon_s v_s W}{A(V_{PO} + 3F_S L_G)}$$

where $F_S$ is the critical electric field for velocity saturation. This model is different from the conventional FET models because the drain current saturation is independent of $V_{GS}$, but at the same drain-to-source voltage. For MESFETs of short gate length where inter-valley scattering and negative differential mobility can not fully manifest themselves, a piece-wise linear or exponential velocity field model can be used without introducing significant error [Higgins, 1980].
Taking channel length modulation effect due to velocity saturation into account, the effective gate length is reduced by $L_S$ (see Fig. 2.1). Shur proposed the following for approximating $L_S$ [Shur, 1985],

$$L_s = \frac{2A}{\pi} \ln \left( \frac{\pi \Delta V}{2F_s A} + \left[ \left( \frac{\pi \Delta V}{2F_s A} \right)^2 + 1 \right]^{1/2} \right)$$

(2.5)

where $\Delta V$ is the voltage drop across the saturated region, and it is approximated by

$$\Delta V \approx (V_{DS} - V_s)K_D.$$  

$K_D$ is $\Delta V / (\Delta V + V_{DOM})$ which is selected to be 0.1. $V_{DOM}$ is the voltage drop across the channel under the extension of the depletion region beyond the gate towards the drain. $V_s$ may be accurately approximated by the equation

$$V_s \approx V_{PO} \alpha \frac{(1 - u_G)}{(\alpha + 1 - u_G)}.$$  

(2.6)

where $\alpha = F_S / V_{PO}$ and $u_G = (V_B - V_G) / V_{PO}$. The transconductance parameter, $\beta$ of Eq. 2.4 is modified by the effective gate length $L_G - L_S$

$$\beta = \frac{2\varepsilon_s V_s W}{A \left[ V_{PO} + 3E_C (L_G - L_S) \right]}.$$  

(2.7)

Equations 2.3, 2.5, 2.6 and 2.7 completely describe the square law model. The square law model has been shown to be an accurate analytical model for MESFETs with low pinch-off voltage ($V_{PO} < 2V$) [Shur, 1985.]

The square law model shows a good correlation to measured data when $V_{GS}$ is near the threshold voltage. However, at higher $V_{GS}$, the reduction in channel height between the channel entrance and the point where the carrier velocity saturates is usually a negligible fraction of the height at the entrance.
is known as the complete velocity saturation model. The complete velocity saturation model assumes all the carriers in the channel are at saturated velocity and the width of depletion layer is the same across the entire channel. The saturation current is proportional to the depletion layer width which follows a square root relationship to $V_{GS}$. The current voltage relationship based on the complete velocity saturation model is

$$ I_{DS0}^{SAT} = q N_D v_{SAT} W A_{DS}, $$  \hspace{1cm} 2.8

where $A_{DS}$ is the depletion width given by

$$ A_{DS} = A \left[ 1 - \left( \frac{V_{BI} - V_{GS}}{V_{P0}} \right)^{1/2} \right]. $$  \hspace{1cm} 2.9

Current in the triode region may be modeled by a similar expression as for the square-law model of Eq. 2.3 except $I_{DS0}^{SAT}$ is replaced by Eq. 2.8.

The series resistances $R_S$ and $R_D$ should also be considered in modeling MESFETs with non self-aligned gate. The actual gate voltage $V_{GS}$ and drain to source voltage $V_{DS}$ in the equations above are

$$ V_{GS} = V_{GS_{TOTAL}} - R_S \cdot I_{DS}, \text{ and } V_{DS} = V_{DS_{TOTAL}} - (R_S + R_D) \cdot I_{DS} $$  \hspace{1cm} 2.10

respectively.

Equations 2.3, 2.5, 2.6 and 2.7 completely describe the square law model and Eq. 2.3, 2.8 and 2.9 describe the complete velocity saturation model.

The output conductance $g_{DS0}$, or $\frac{\partial I_{DS}}{\partial V_{DS}}$, at one constant $V_{GS}$ based on both models is

$$ g_{DS0} = I_0 \left[ (1 + \lambda V_{DS}) \alpha \text{sech}^2(\alpha V_{DS}) + \lambda \tanh(\alpha V_{DS}) \right]. $$  \hspace{1cm} 2.11

where $I_0$ is $\beta(V_{GS} - V_T)^2$ for the square law model and $I_0$ is $I_{SAT}$ for the complete velocity saturation model.
Non-Isothermal Analytical Model

Thermal effects may be an important contribution to the electrical characteristics of a GaAs MESFET because of the lower thermal conductivity of GaAs. The analytical models presented in the previous section do not take into account the electro-thermal effects. To account for electro-thermal effects in GaAs MESFETs, Canfield et al. [Canfield, 1990] modified the basic Curtice model to include a temperature dependent mobility. The electron mobility is assumed to be inversely proportional to temperature given by

\[ \mu(T) = \frac{\mu_0}{1 + \delta T/T_0}, \] 2.12

where \( T_0 \) and \( \mu_0 \) are the heat sink temperature and its corresponding mobility, and \( \delta T \) is the average temperature rise in the channel. The average channel temperature can be approximated by applying the concept of thermal resistance based on the assumption of an isothermal active channel.

The three modes of heat transfer in thermal analysis are conduction, convection and radiation. Heat conduction is the transfer of heat from higher-temperature to lower-temperature through a solid medium. This mechanism is responsible for heat transfer inside the MESFET. The thermal conductivity equation under steady state conditions for the governing temperature, \( T \), at a position \( (x,y,z) \) in a semiconductor device is

\[ \nabla \cdot k(T) \nabla T = -q \] 2.13

where \( k(T) \) is the nonlinear thermal conductivity and \( q(x,y,z) \) is the heat generation per unit volume at that point. The thermal conductivity \( k(T) \) is a nonlinear function because of the various temperature dependent mechanisms responsible for heat conduction in the semiconductor material. At very low temperature (less than 40K), the thermal conductivity of GaAs increases sharply with increasing
temperature due to the specific heat of the material. At temperatures higher than 600K, electron–hole pairs and photons contributes significantly to thermal conduction. In the temperature regime of normal GaAs MESFET operation, the thermal conductivity \( k(T) \) of GaAs is dominated by phonon scattering, and can be modeled empirically by

\[
k(T) = 44\left(\frac{T}{300}\right)^{-1.25} \text{ (W/m°C)}.
\]

Because of the nonlinear thermal conductivity, a direct solution of Eq. 2.13 is difficult. Assuming the device has an isotropic uniform heatsink, the nonlinear heat equation can be reduced to a linearized boundary condition problem of the transformed variable \( \tau \) [Joyce, 1975]. The linearized temperature, \( \tau \), is associated with the actual temperature \( T \) by Kirchoff's transformation

\[
\tau(T) = T_0 + \frac{1}{k_0} \int_{T_0}^{T} k(T) dT,
\]

where \( T_0 \) and \( k_0 \) are heat sink temperature and thermal conductivity respectively. The gradient and divergence of Eq. 2.13 are

\[
k_0 \nabla \tau = k \nabla T,
\]

and

\[
k_0 \nabla^2 \tau = \nabla \cdot k \nabla T.
\]

Equation 2.16 shows both variables \( T \) and \( \tau \) have the same boundary value of \( T_0 \), while Eq. 2.17 shows that the variable \( \tau \) satisfies the linear heat flow equation, although \( T \) does not. The solution of \( T \) can be obtained by first solving the linearized heat equation (Eq. 2.16) for \( \tau \), then take the inverse transform for \( T \).
Applying this technique to solve for temperature $T$ of an isothermal channel, first let $\tau_1$ be the difference between linearized temperature $\tau$ and $T_0$

$$\tau_1 = \tau(T) - T_0 = \frac{1}{k_0} \int_{T_0}^{T} k(T')dT'$$  \hspace{1cm} 2.18

The solution of $\tau_1$ can be approximated by assuming the MESFET is a half-cylindrical heat source with diameter $D$ and width $W$ resting on the surface of a substrate of thickness $t_{\text{SUB}}$. Further assume $D \ll t_{\text{SUB}}$ and $D \ll W$ [Wemple, 1982]

$$\tau_1 = \frac{P_{T_0}}{\pi k_0 W} \ln \frac{8t_{\text{SUB}}}{\pi D}$$  \hspace{1cm} 2.19

where $P_{T_0}$ is equal to $I_{DS0}V_{DS}$. The actual temperature difference $\delta T$ can be found by applying Kirchhoff’s transformation to the solution of the linearized equation above [Canfield, 1990]

$$\frac{\delta T}{T_0} = \frac{1 - (1 - P_{T_0}/4P_0)^4}{(1 - P_{T_0}/4P_0)^4}$$  \hspace{1cm} 2.20

where $P_0$ is a constant given by

$$P_0 = \frac{\pi k_0 W T_0}{\ln(8t_{\text{SUB}}/\pi L_G)}$$  \hspace{1cm} 2.21

Notice in Eq. 2.22, the effective width of the heat source $D$ is replaced by the length of the gate. The drain current voltage relationship given by Eq. 2.3 is modified by the temperature dependent mobility given by Eq. 2.12 and Eq. 2.20.

$$I_{DS}(T) = I_{DS0} \frac{1}{1 + \delta T/T_0} (1 + \lambda V_{ds}) \tanh(\alpha V_{ds})$$  \hspace{1cm} 2.23

The temperature dependent output conductance is thus,
Other heat transfer mechanisms may also affect the overall temperature of a MESFET. Examples are heat transfer due to convection and radiation. Without external forces, such as a fan, natural convection and radiation are assumed to have negligible affect on the overall temperature of the device, thus are ignored in the analytical model. Also ignored are conduction through the drain, source and gate contacts.

Several assumptions made in this model may lead to inaccurate results. First, the power distribution is not uniform within the channel. The localized heat sources within the channel increases the overall channel temperature. Second, in Canfield's derivation, the channel is modeled as a half cylindrical heat source with diameter $L_G$. In an actual device, the effective width of the heat source can only be found empirically. Wemple and Hwang [Wemple, 82] has found that direct replacement of the diameter $D$ of Eq. 2.20 by the gate length does not model the channel temperature accurately. They have shown by the measurement on a 2um gate length MESFET, that $D$ is best modeled by $2L_G$. Another assumption made is that all the temperature effects appear in the mobility (see Eq. 2.12). No account was given to temperature dependence of the saturation velocity.
Figure 2.1  Depletion region and current saturation under different biased conditions.

Figure 2.2  Simplified piece-wise linear velocity-field relationship.
Chapter Three
TWO DIMENSIONAL SIMULATION

Basic Equations

The static and dynamic behavior of carriers in semiconductor devices under external fields can be described approximately by the drift—diffusion model. The equations of this model are classified into Maxwell equations, the current density equations and the continuity equations. Under steady state operation and no external magnetic field, only two of the six Maxwell equations determine operation of a device

\[ \mathbf{D} = \varepsilon_s \mathbf{E} \]  \hspace{1cm} 3.1

\[ \nabla \cdot \mathbf{D} = \varrho(x, y, z) \]  \hspace{1cm} 3.2

where \( \mathbf{D} \) is field displacement vector, \( \varepsilon_s \) is the dielectric permittivity, \( \mathbf{E} \) is the electric field and \( \varrho \) is charge density. The two equations above can be combined into Poisson's equation for the electrostatic potential \( \psi \)

\[ \nabla^2 \psi = -\frac{\varrho}{\varepsilon_s} . \]  \hspace{1cm} 3.3

The charge density \( \varrho \) is composed of the electron and hole free carrier densities and the net concentration of positively charged ionized impurities

\[ \varrho = q(p - n + C) . \]  \hspace{1cm} 3.4

Since an \( n \)-type MESFET is a majority carrier device, the concentration of free carriers in the active channel due to holes is negligible in comparison to that of electrons. With this assumption, Poisson's equation expressed in two dimensional form simplifies to

\[ \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \frac{q}{\varepsilon_s} (n - C) , \]  \hspace{1cm} 3.5
where \( C = N_D^+ \).

The continuity equations for electrons and holes are

\[
\frac{\partial p}{\partial t} = -G_p + U_p + \frac{1}{q} \nabla \cdot J_p \tag{3.6}
\]

\[
\frac{\partial n}{\partial t} = G_n - U_n + \frac{1}{q} \nabla \cdot J_n \tag{3.7}
\]

where \( G_n, G_p, U_n \) and \( U_p \) are the generation and recombination rates for electrons and holes respectively. With the same assumption of negligible hole concentration, we can neglect the continuity equation for holes in an n-type MESFET. Without external generation and recombination, the recombination effect may be neglected, even if minority carriers are taken into account. Therefore, under steady state conditions, Eq. 3.7 reduces to

\[
\frac{\partial J_{nx}}{\partial x} + \frac{\partial J_{ny}}{\partial y} = 0 \tag{3.8}
\]

The current density vector for electrons is composed of drift and diffusion components caused by the electric field and carrier concentration gradient

\[
J_n = q\mu_n E + qD_n \nabla n \tag{3.9}
\]

where \( \mu_n \) is electron mobility and \( D_n \) is diffusion constant which is equal to \((kT/q)\mu_n\) by the Einstein relationship. Eq. 3.9 expressed in two dimensional form becomes

\[
J_{nx} = -q(\mu_n \frac{\partial \psi}{\partial x} - D_n \frac{\partial n}{\partial x}) \tag{3.10}
\]

\[
J_{ny} = -q(\mu_n \frac{\partial \psi}{\partial y} - D_n \frac{\partial n}{\partial y}) \tag{3.11}
\]

A complete quasi-static model of an n-type MESFET under steady state operation can be described by Poisson's equation, the continuity equation, the
current density equation, and heat equation, which are Eqs. 3.5, 3.8, 3.10, 3.11 and 2.13 respectively.

As described earlier, the electron velocity and electric field relationship deviates from the proportional constant, $\mu_n$, at high field. Due to the transferred electron effect in GaAs, the velocity–field relationship shows velocity overshoot. A common empirical equation used to model velocity field relationship in GaAs MESFET is [Ruch, 1970]

$$\mu_n(E) = \mu_{n0} \frac{1 + \frac{\nu_{sat}(E)}{\mu_{n0}|E|} \left(\frac{E}{E_0}\right)^4}{1 + \left(\frac{E}{E_0}\right)^4}.$$  \hspace{1cm} 3.12

Because of the stable negative resistance (SNR) or Gunn oscillations caused by the transferred electron effect, one needs to consider the finite substrate current in the semi insulating substrate in order to accurately model a GaAs MESFET using this mobility model. The boundary between the SNR and positive conductance (pentode–like) operation for a GaAs MESFET assuming no substrate current is defined by the two conditions [Yamaguchi, 1976]

$$n \cdot L_{gd} > 1 \times 10^{12} \text{ cm}^{-2}$$

and

$$n \cdot d > 2 \times 10^{11} \text{ cm}^{-2}.$$  \hspace{1cm} 3.13

Simulation without taking into account of the substrate may result in Gunn oscillation or stable negative resistance not observed in an actual device [Wada, 1979]. In an actual device, the finite substrate conduction reduces the effect of the Gunn domain. With substrate conduction, the boundary between these operating regions has been shown both experimentally and numerically to be less stringent [Yamaguchi, 1976]
As discussed in the Introduction, the purpose of the present work is to study the negative conductance due to self heating in the active channel of GaAs MESFETs. For simplicity the channel is uniformly doped and no EL2 traps or substrate current are considered. The device geometry and donor concentration have been selected so that $I_{DS}$ is sufficiently large to cause a significant channel temperature variation. For a 1$\mu$m gate length and 0.2$\mu$m channel depth and $N_D$ of $6.4 \times 10^{16}$ cm$^{-3}$, the MESFET is found to be operating in the SNR region as shown by the two conditions mentioned in Eq. 3.13. In an actual device of similar geometry, no SNR was observed. To accurately model this device using the overshoot velocity model, one would need to consider substrate current. Without adding to the complexity of the simulation program, a simple exponential velocity model which accounts for velocity saturation but not the transferred electron effect is used (see Fig. 3.1)

$$\mu_n(E) = \frac{v_{nsat}}{E} \left[ 1 - \exp\left(\frac{u_{n0}E}{v_{nsat}}\right) \right]. \tag{3.14}$$

Both the saturation velocity and low-field mobility have a $1/T$ dependence on temperature. The temperature variation of these two variables are represented empirically by [GATEs, 1988]

$$\mu_n(T) = \mu_n(T_0) \left(\frac{T}{300}\right)^{-2.3} \left(\frac{m}{V_S}\right). \tag{3.15}$$

$$v_{nsat} = (0.64 + 1.38\mu_n - 0.82\mu_n^2) * 1E5 \left(\frac{m}{S}\right). \tag{3.16}$$

Neglecting the finite substrate current, simulation of Poisson's equation and the continuity equation require only the channel region. The heat equation must be modeled for both the channel and the nonconductive substrate. The geometry of the simulated device is shown in Fig. 3.2.
Linearization And Discretization

Two different numerical methods, finite element and finite difference, may be used to solve the full set of semiconductor partial differential equations described in the previous section. Three basic steps are required for solving semiconductor devices using either numerical methods. First, the simulation region is divided into subdomains suitable for the type of numerical scheme selected. Secondly, each of the independent variables in the semiconductor equations are mapped to a discrete point in a subdomain by approximating the original partial differential equations by either a shape function or a difference quotient as in the case of the finite-element or the finite-difference method respectively. With proper boundary conditions, the last step is to obtain a solution to the approximated equations at each discrete points. Although it is not possible to obtain an exact solution to the original partial differential equations using this technique, careful planning of all three steps above can produce a good approximation. Finite-elements methods provide versatility in defining the shapes and sizes of the simulation mesh. However, because it requires a greater degree of programming complexity, it is less commonly used. For devices with geometries suitable for implementation of a rectangular mesh, the finite-difference method has been found to be easier to implement as it produces systems of equations with sparse matrices with only a few non-zero diagonal. The disadvantages of the finite-difference technique are reduced order of accuracy, numerically degenerate long-shaped rectangles, and computational overhead in the equation setup [Reiser,1971].

The numerical scheme chosen to solve this set of differential equations in the present work is the finite-difference method. The simplest way of dividing the simulation region into subdomains suitable for finite-difference
implementation is the use of a rectangular mesh where the rows and columns are parallel to the x and y-axis. The grid spacing in the mesh is proportional to the number of discrete equations to be solved and the accuracy of the result. The mesh spacing should be chosen to provide numerical stability and should be less than the Debye length

$$L_D = \sqrt{\frac{\varepsilon_0 k T}{q^2 N_D}}.$$  \hspace{1cm} 3.17

Large grid spacings would result in smaller number of grid points, and thus a fewer number of discrete equations to be solved. A smaller grid spacing produces more accurate results at the expense of more computational time. A non-uniform rectangular mesh is most suitable for this type of simulation because it allows finer grids within regions where the variables change the most, such as under the gate, and larger grids in less critical regions such as the substrate. Once the mesh is created, the next step is to map the differential equations to each mesh points.

The discretization scheme selected is the classical five-point method where each of the four independent variables at a mesh point is represented by difference quotients composed of the point itself and its four nearest neighbors. A sample mesh point at i-th row and j-th column of the mesh is shown in Fig. 3.3. Once discretized using five-point center difference scheme, all three equations, Poisson’s, continuity for electrons and heat equation can be expressed in the form

$$B_{ij}u_{i,j-1} + D_{ij}u_{i-1,j} + E_{ij}u_{ij} + F_{ij}u_{i+1,j} + H_{ij}u_{i,j+1} = q_{ij}$$ \hspace{1cm} 3.18

where \( u \) is the variable, and \( B_{ij}, D_{ij}, E_{ij}, F_{ij}, H_{ij} \) and \( q_{ij} \) are constants. For \( N \) mesh points, three sets of \( N \) discretized equations are formed.
Two different methods can be used to solve these equations. The direct Newton's method has a high convergence rate, however it is seldom used because all three equations have to be solved simultaneously, and the resulting coefficient matrix is an irregular sparse matrix which is difficult to solve. Since N is usually large, direct Gaussian elimination is not feasible. Alternatively, modified Newton’s methods which have slower convergence rate but produce smaller and more regular coefficient matrices are primarily used.

Gummel has shown that for systems which are not strongly coupled, the device equations may be decoupled, and solved independently and iteratively until convergence occurs. To assist the overall convergence rate, Gummel has proposed an alternate form of the Poisson’s equation based on Newton’s method

\[ \nabla \cdot \nabla \psi - \frac{q}{\varepsilon_s} \left( \frac{\partial n}{\partial \psi} - \frac{\partial C}{\partial \psi} \right) \psi = - \nabla \cdot \nabla \psi_0 + \frac{q}{\varepsilon_s} (n - C) \tag{3.19} \]

where \( \psi_0 \) is the initial approximation and \( \psi = \psi_0 + \partial \psi \). Eq. 3.19 can be linearized by assuming electron concentration is of the form \( n = \phi_n \exp(\psi/V_{th}) \). Thus \( \partial n/\partial \psi = n/V_{th} \). Placed in the iterative form where \( \partial \psi = \psi^{k+1} - \psi^k \), Eq. 3.19 becomes

\[ \nabla \cdot \nabla \psi^{k+1} = \frac{q}{\varepsilon_s} \left[ \frac{n^k}{V_{th}} (\psi^{k+1} - \psi^k) + (n^k - C) \right] \tag{3.20} \]

where \( k \) is Gummel’s iteration number. Next, the continuity equation for electrons is solved based on the new potential \( \psi^{k+1} \) and previous temperature \( T^k \). Lastly, the heat equation is solved using \( \psi^{k+1} \) and \( n^{k+1} \). The above procedure corresponds to the completion of one Gummel’s loop. This process repeats itself until the change in \( \psi, n \) and \( T \) between the \( k \)-th and the \( (k+1) \)-th iteration is less
than a predefined tolerance value. A flow chart of Gummel's algorithm is shown in Fig. 3.4.

Applying the standard five-point center-difference discretization method to Poisson's equation at the location of the i-th column and the j-th row produces the difference equation

\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \frac{-q}{\varepsilon} (n_{ij} - C_{ij})
\]

which is equal to

\[
\psi_{i-1,j} - \psi_{i,j} + \psi_{i+1,j} + \psi_{i,j-1} + \psi_{i,j+1} = \frac{q}{\varepsilon} (n_{ij} - C_{ij})
\]

Discretization of the continuity equation is much more crucial than Poisson's equation. Several techniques have been used by various authors, such as direct discretization of continuity equation in variable \( n \) [Reiser, 1971] or logarithmic variable [Slotboom, 1969]. It has been shown both techniques lead to gross errors in case of large voltage drops over a single mesh cell, e.g. \( \delta \psi > 2kT/q \). A superior method which does not have such limitation was introduced by Scharfetter and Gummel [Scharfetter, 1969]. Four assumptions are made in the derivation:
1. The Einstein relation holds for the mobility and diffusivities
2. The current density is constant within the mesh cell
3. Constant partial derivatives of $\psi$ and $E$ along integration path
4. Constant mobility and diffusivities along integration path

Instead of discretizing the continuity equation directly, an expression is first obtained for the carrier concentration by integrating the current density equation over the mesh cell

$$\mu_n \frac{\partial \psi}{\partial x} - D_n \frac{\partial n}{\partial x} = J_{n_{x_i+1/2,j}} + \left( x - x_i - \frac{h_i}{2} \right) \cdot \frac{\partial J_{nx}}{\partial x_{i+1/2,j}},$$

yielding electron current density at the mesh point $(i+1/2,j)$

$$J_{n_{x_{i+1/2,j}}} = D_{n_{i+1/2,j}} \frac{B\left(\psi_{i,j} - \psi_{i+1,j} \right)}{h_i} n_{i,j} - B\left(\psi_{i+1,j} - \psi_{i,j} \right) n_{i+1,j}$$

where $B(x)$ is the Bernoulli function which is defined as

$$B(x) = \frac{x}{e^x - 1}.$$

The carrier diffusivity and mobility at mid intervals can be approximated using linear interpolation

$$D_{n_{i+1/2,j}} = \frac{D_{n_{i,j}} + D_{n_{i+1,j}}}{2}$$

$$\mu_{n_{i+1/2,j}} = \frac{\mu_{n_{i,j}} + \mu_{n_{i+1,j}}}{2}.$$

Substitute discretized equations of $J_{nx}$ into continuity equation for electrons and collect like terms we get

$$n_{i,j} D_{n_{i,j}} B\left(\frac{\psi_{i,j} - \psi_{i,j}}{U_T} \right) h_{i,j} + n_{i-1,j} D_{n_{i-1,j}} B\left(\frac{\psi_{i-1,j} - \psi_{i,j}}{U_T} \right) k_{i,j} + k_j$$
\[-n_{ij}D_{n_{ij-1/2}} \left( \frac{\psi_{ij} - \psi_{ij-1}}{U_T} \right) \frac{h_{i-1} + h_i}{2k_{j-1}} + D_{n_{ij-1/2}} \left( \frac{\psi_{ij} - \psi_{i-1,j}}{U_T} \right) \frac{k_{j-1} + k_j}{2h_{i-1}} \]

\[+ D_{n_{ij+1/2}} \left( \frac{\psi_{ij} - \psi_{i+1,j}}{U_T} \right) \frac{k_{j-1} + k_j}{2h_i} + D_{n_{ij+1/2}} \left( \frac{\psi_{ij} - \psi_{ij+1}}{U_T} \right) \frac{h_{i-1} + h_i}{2k_j} \]

\[+ n_{i+1,j}D_{n_{i+1,j}} \left( \frac{\psi_{i+1,j} - \psi_{ij}}{U_T} \right) \frac{k_{j-1} + k_j}{2h_i} + \]

\[+ n_{i,j+1}D_{n_{i,j+1/2}} \left( \frac{\psi_{ij+1} - \psi_{ij}}{U_T} \right) \frac{h_{i-1} + h_i}{2k_j} = 0 . \quad 3.27 \]

Consider the heat transport Eq. 2.13 in its two dimensional form with the nonlinear thermal conductivity replaced by Eq. 2.14

\[\frac{\partial}{\partial x} \left( K_0 T^{-5/4} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_0 T^{-5/4} \frac{\partial T}{\partial y} \right) = -J \cdot E . \quad 3.28 \]

Rearranging the equation above

\[-4K_0 \left[ \frac{\partial^2}{\partial x^2} (T^{-1/4}) + \frac{\partial^2}{\partial y^2} (T^{-1/4}) \right] = -J \cdot E . \quad 3.29 \]

Substitute the variable \( u \) for \( T^{-1/4} \)

\[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{J \cdot E}{4K_0} . \quad 3.30 \]

The discretized form of the heat equation is thus

\[u_{i,j-1} \frac{h_{i-1} + h_i}{2k_{j-1}} + u_{i-1,j} \frac{k_{j-1} + k_j}{2h_{i-1}} \]

\[- u_{i,j} \left( \frac{h_{i-1} + h_i}{2k_{j-1}} + \frac{k_{j-1} + k_j}{2h_{i-1}} \right) \]

\[- \frac{k_{j-1} + k_j}{2h_i} + \frac{h_{i-1} + h_i}{2k_j} \]
where $K_0$ is equal to $44/300^{-1.25}$ W/m°C. Equations 3.22, 3.27, and 3.31 are the discretized Poisson’s, continuity and heat transport equations of an internal mesh point. With the difference equations defined for the internal mesh points, the next step is to setup the boundary conditions for the initial—value problem.

Boundary Conditions

Consider the cross section of an n—type MESFET shown in Fig. 3.5, the boundaries A–B, B–C, C–D, A–E and D–F are the physical boundaries while all others are introduced as artificial boundaries separating devices. Four types of boundaries are included in this device — Ohmic, Schottky, free surface and artificial boundary.

Ohmic contact corresponds to A–E and D–F. The electrostatic potential of a voltage controlled Ohmic contact is

$$\psi_{\text{Ohmic}} = \psi_{\text{bi}} + \psi_D$$

where $\psi_D$ is the external applied bias, and $\psi_{\text{bi}}$ is the built—in potential referenced at the intrinsic level

$$\psi_{\text{bi}} = \frac{kT}{q} \ln \left( \frac{C}{n_i} \right) .$$

The carrier concentration at the Ohmic contacts can be obtained assuming infinite surface recombination and vanishing space charge which defines Eq. 3.34 and Eq. 3.35
\[ np - n_i^2 = 0 \quad 3.34 \]
\[ n - p - C = 0. \quad 3.35 \]

The two assumptions above form Dirichlet boundary condition for the electrons

\[ n = \frac{\sqrt{C^2 + 4n_i^2 + C}}{2}. \quad 3.36 \]

For the case of an n-type MESFET where the shallow donor concentration is much greater than the acceptor concentration and intrinsic concentration, Eq. 3.36 becomes

\[ n \approx N_D^+ = N_D. \quad 3.37 \]

Eq. 3.33 and Eq. 3.37 define the electrostatic potential and electron concentration at the Ohmic contacts. Both boundary conditions for \( \psi \) and \( n \) at the Ohmic contacts are Dirichlet boundary conditions where each of the independent variables are constants.

The second type of boundary is a Schottky contact which corresponds to B–C of Fig. 3.5. Assuming no Schottky barrier lowering effect, the electrostatic potential can be treated as a Dirichlet boundary with a constant potential described by

\[ \psi_{\text{Schottky}} = \psi_{\text{bi}} + \psi_D - \psi_B. \quad 3.38 \]

\( \psi_{\text{bi}}, \psi_D, \) and \( \psi_B \) are the built-in potential, the external applied gate bias, and the Schottky gate barrier height referenced at the intrinsic level respectively. The barrier height for GaAs is around 0.8eV. To simulate the Schottky gate on an n-type GaAs MESFET, Laux used Dirichlet boundary conditions to model the electron concentration [Selberherr, 1984]. Depending on the gate bias, two different equations can be used to define the electron concentration.
\[ n = N_c \exp \left( \frac{q}{kT} (\psi_D - \psi_B) \right) \quad \text{if } \psi_D \geq 0 \]

\[ n = \frac{N_c \exp \left( \frac{-q\psi_B}{kT} \right)}{14 \sqrt{\frac{q}{kT} (\psi_B - \psi_D)} - \ln \frac{N_c}{N_0} + 1} \quad \text{if } \psi_D < 0 \]  

3.39

This model is chosen over the thermionic emission theory [Sze, 254, 1981] in the actual implementation, because Dirichlet boundary conditions are numerically less sensitive to spacing than Neuman boundaries.

The third type of boundary is that of a free surface. Neglecting surface states, one can use Neuman boundary conditions for zero current conduction across such surfaces. The method of handling such boundaries is identical to the fourth type of boundary — artificial boundary — which corresponds to E—F, H—G, H—E and G—F of Fig. 3.5. Assuming that the device simulated is self-contained and without influence from adjacent devices, the gradients of all independent variables normal to these surfaces are set to zero

\[ \frac{\partial \psi}{\partial n} = 0 , \quad \frac{\partial n}{\partial n} = 0 , \quad \frac{\partial T}{\partial n} = 0 . \]  

3.40

In the case of modified heat equation, where T is replaced by \( u^{-4} \), the boundary condition \( \frac{\partial T}{\partial n} = 0 \) implies \( \frac{\partial u}{\partial n} = 0 \). The electrostatic potential and carrier concentrations of a mesh point on the free surfaces or the artificial boundaries can not be expressed simply by the classical five-point method described previously because it does not have all four neighboring points. Instead, a reflection technique is used to discretize such equations. By applying the reflection technique and the center-difference method to a point along the F—H artificial boundary gives the relationships

\[ \frac{\partial \psi}{\partial n_{i+1/2,j}} = -\frac{\partial \psi}{\partial n_{i-1/2,j}} \]
Based on the relationships given in Eq. 3.41, the discretized forms of the Poisson's, continuity and heat transport equations are

\[
\begin{aligned}
\psi_{i,j-1} \frac{h_{i-1}}{k_{j-1}} + \psi_{i,j} \frac{k_{j-1} + k_j}{h_{i-1}} - \psi_{i,j} \left( \frac{h_{i-1}}{k_{j-1}} + \frac{k_{j-1} + k_j}{h_{i-1}} \right) \\
+ \psi_{i,j+1} \frac{h_{i-1}}{k_j} = -\frac{q}{\varepsilon_s} (n_{i,j} - C_{ij}) h_{i-1} \frac{k_{j-1} + k_j}{2},
\end{aligned}
\]

\[3.42\]

\[
\begin{aligned}
\begin{aligned}
n_{i,j-1} D_{n_{i-1/2}} B \left( \frac{\psi_{i,j-1} - \psi_{i,j}}{U_T} \right) \frac{h_{i-1}}{k_{j-1}} + n_{i-1,j} D_{n_{-1/2}} B \left( \frac{\psi_{i-1,j} - \psi_{i,j}}{U_T} \right) \frac{k_{j-1} + k_j}{h_{i-1}} \\
- n_{i,j} \left[ D_{n_{i-1/2}} B \left( \frac{\psi_{i,j} - \psi_{i,j-1}}{U_T} \right) \frac{h_{i-1}}{k_{j-1}} + D_{n_{-1/2}} B \left( \frac{\psi_{i,j} - \psi_{i-1,j}}{U_T} \right) \frac{k_{j-1} + k_j}{h_{i-1}} \\
+ D_{n_{i+1/2}} B \left( \frac{\psi_{i,j} - \psi_{i,j+1}}{U_T} \right) \frac{h_{i-1}}{k_j} \right] \\
+ n_{i,j+1} D_{n_{i+1/2}} B \left( \frac{\psi_{i,j+1} - \psi_{i,j}}{U_T} \right) \frac{h_{i-1}}{k_j} = 0,
\end{aligned}
\end{aligned}
\]

\[3.43\]

\[
\begin{aligned}
\begin{aligned}
u_{i,j-1} \frac{h_{i-1}}{k_{j-1}} + \nu_{i-1,j} \frac{k_{j-1} + k_j}{h_{i-1}} - \nu_{i,j} \left( \frac{h_{i-1}}{k_{j-1}} + \frac{k_{j-1} + k_j}{h_{i-1}} \right) \\
+ \nu_{i,j+1} \frac{h_{i-1}}{k_j} = \left( \frac{J_{nx,i} E_{x,i} + J_{ny,i} E_{y,i}}{4K_0} \right) \frac{h_{i-1}}{2} \frac{k_{j-1} + k_j}{2}
\end{aligned}
\end{aligned}
\]

\[3.44\]

respectively.

Similar expressions can also be obtained for artificial boundary points along A–B, C–D, E–G, F–H and E–F.
Stone's Implicit Method

With the proper boundary conditions applied, the three separate systems of difference equations based on Eqs. 3.22, 3.27 and 3.31 define the electrical and thermal behaviors of the GaAs MESFET. The most direct method of solving a set of discretized equations is by Gaussian elimination. This technique, however, is not feasible for a system with large number of unknowns because it requires $2^N$ arithmetic operations to solve $N$ equations. For simulation of semiconductor devices, this method would require both long computational time and massive storage because $N$ is usually in the hundreds. A more suitable alternative is an iterative method. To solve each system of equations, we can take the advantage of equations discretized using the five-point scheme. For each set of equations, the natural ordering by row starting from the left and bottom most point $j=0$ and $k=0$ as shown in Fig. 3.5, the equations are ordered by first ascending $j$, then ascending $k$. This ordering yields coefficient matrix of rank $N$ with five non-zero diagonals in the form as shown in Fig. 3.6, where $m$ is number of columns and $n$ is number of rows. Instead of direct Gaussian elimination, special techniques should be used to solve such sparse matrix to avoid storing and calculating the zero elements. The iterative method chosen for solving Poisson's, the continuity and heat equations was developed by Herbert Stone [Stone, 1968]. Stone has shown his strongly implicit method has a higher convergence rate than the Point-Jacobi, over-relaxation, and alternate direction iteration methods.

Starting with the original system of equations,

\[ M \cdot u = q, \]  \hspace{1cm} 3.45

where $u$ and $q$ are the variables and right hand side vectors respectively, and $M$ is the five diagonal coefficient matrix of rank $N$ (where $N$ is the number of mesh points) the first step is to arrange the system of equations into a form suitable for
matrix factorization. The next step is to replace $M$ with a modified matrix, $M'$, that can be factored into an upper and a lower triangular matrices, $L$ and $U$, with each matrix having only three non-zero elements in each row

$$M' = L \cdot U = (M + A) .$$

The computational time of solving this matrix should be proportional to $N$ instead of $2^N$ as in Gaussian elimination. $M'$, designated as $(M + A)$, has to be a close approximation of the original matrix, $M$, and is both easily factorable and has a good convergence rate.

Based on this technique the modified equation in $M' \cdot u = (L \cdot U) \cdot u = q$ at the point $(j,k)$ expressed in terms of the coefficients of $L$ and $U$ is

$$b_{ij} u_{ij-1} + b_{ij} e_{ij-1} u_{i+1,j-1} + c_{ij} u_{i-1,j}$$
$$+ \left( d_{ij} + b_{ij} f_{ij-1} + c_{ij} e_{i-1,j} \right) u_{ij}$$
$$+ d_{ij} e_{ij} u_{i+1,j} + c_{ij} f_{i-1,j} u_{i-1,j+1} + d_{ij} f_{ij} u_{i,j+1} = q_{ij} .$$

This resulting product matrix has seven diagonals, five of which are from the original matrix $M$. Two other diagonals correspond to points $u_{j-1,k+1}$ and $u_{j+1,k-1}$.

To eliminate the effect of these two extra terms, Stone demonstrated the variable $u$ at these two additional points can be approximated by

$$u_{i-1,j+1} \approx - u_{ij} + u_{ij+1} + u_{i-1,j}$$
$$u_{i+1,j-1} \approx - u_{ij} + u_{i+1,j} + u_{ij-1} .$$

using a Taylor series expansion. These relations are close approximations if the spacings between grid points are small. For additional flexibility, a variable iteration parameter, $\alpha$, is introduced to help the convergence rate. The original
form of Eq. 3.18 is modified to include the two extra points, and then canceling the effect of these two points by the relationships of Eq. 3.48

\[ B_{ij} u_{ij-1} + D_{ij} u_{i-1,j} + E_{ij} u_{ij} + F_{ij} u_{i+1,j} + H_{ij} u_{ij+1} + C_{ij} F_{ij} 1.11+1d ± Hid Uid+1 + Cid \]

\[ G_{ij} [u_{i+1,j-1} - \alpha (-u_{ij} + u_{i+1,j} + u_{ij-1})] = q_{ij}. \] 3.49

Collecting like-terms, the coefficients of Eq. 3.47 can be matched to the coefficients of Eq. 3.49

\[ b_{ij} = B_{ij} - \alpha C_{ij} \]
\[ b_{ij} e_{ij-1} = C_{ij} \]
\[ c_{ij} = D_{ij} - \alpha G_{ij} \]
\[ d_{ij} + b_{ij} f_{ij-1} + c_{ij} e_{ij-1,j} = E_{ij} + \alpha C_{ij} + \alpha G_{ij} \]
\[ d_{ij} e_{ij} = F_{ij} - \alpha C_{ij} \]
\[ d_{ij} f_{ij} = H_{ij} - \alpha G_{ij} \] 3.50

This set of six relations in Eq. 3.50 defines the modified matrix \( M' \) which is both factorable and approximates the original matrix \( M \). Eq. 3.45 is further modified to a form suitable for an iterative scheme

\[ M' \delta^{n+1} = LV^{n+1} = R^n \] 3.51

where

\[ \delta^{n+1} = (u^{n+1} - u^n), \quad V^{n+1} = U\delta^{n+1}, \quad \text{and} \quad R^n = (q - Mu^n), \]

and \( n \) is the iteration number.

The solution of \( u^n \) is obtained by first finding intermediate coefficients \( b, c, d, e, f, R \) and \( V \) for every mesh point starting from \( j=0 \) with \( i \) taking on the values
of 0, 1, 2 ..., I. Then j is incremented by 1. The vector V is obtained by the relationship

\[ b_{ij} V_{i,j-1} + e_{ij} V_{i-1,j} + d_{ij} V_{i,j} = R_{i,j}^{n} \]  

3.52

of the lower tri-diagonal matrix. Once all the intermediate coefficients are obtained, the vector \( \delta^{n+1} \) is solved in the reverse order using the relationship

\[ \delta_{ij}^{n+1} + e_{ij} \delta_{i-1,j}^{n+1} + f_{ij} \delta_{ij}^{n+1} = V_{ij} \]  

3.53

of the upper tri-diagonal matrix.

Stone's iteration terminates when the maximum change in variable \( u \), or the maximum \( \delta \) is less than a predefined use value.

Initial Guess

As with any numerical method, the starting value of the iteration is important both to the rate of convergence and in some cases may determine whether the simulation will converge at all. In order to generate a family of characteristic curves using the present simulation program, one begins by selecting a constant applied gate bias, \( V_{GS} \), then varies the applied drain bias \( V_{DS} \) starting from 0. Except for a change in \( V_{GS} \), the initial guesses of \( \psi \), \( n \) and \( T \) for each successive change in \( V_{DS} \) are generated from the two dimensional solution obtained from the previous \( V_{DS} \). \( V_{GS} \) is updated when the IV curve for the current \( V_{GS} \) is completed. Two types of initial guesses are implemented in the present simulation program. The first is a one dimensional solution used for each new gate bias. The second is an interpolation method for each change in the applied drain bias.

At the beginning of a new gate bias, a routine for solving one dimensional Poisson's and continuity equations is used to generate solutions of the potential \( \psi \) and the carrier concentration \( n \) for two vertical structures. Representing a
vertical strip from the gate to the channel—substrate interface is a Shottky diode structure with the applied gate bias and the boundary conditions given by Eqs. 3.35 and Eq. 3.36. Representing a strip from the free surface to the channel—substrate contact is another diode structure. The technique for solving one dimensional Poisson's and continuity equations using Gummel's algorithm are well documented [Klopfenstein, 1975]. Once the one dimensional solution for the electrostatic potential and carrier concentration are obtained, the values of $\psi$ and $n$ of the Schottky diode are mapped across the gate region as the initial guess, and the solution of the second one-dimensional structure is mapped across everywhere else. Since $V_{DS}$ is always selected to be 0V at the beginning of each new $V_{GS}$, the initial guess for the temperature at each mesh point is set to be the substrate temperature $T_0$.

The second type of initial guess is used at the beginning of each successive change in the applied drain bias. Because most of the potential drop is under the gate region, updating the potential at the drain contact with each change in $V_{DS}$ results in slow convergence or may cause divergence if the change in $V_{DS}$ is too large. The new guess is setup with the knowledge that the majority of potential drop will be under the gate, and not in the drift regions where the series resistance is minimal. The change in $V_{DS}$, $\delta V_{DS}$, is thus distributed in the region under the gate based on the equation

$$\psi_{ij}^0 = \psi_{ij}^{-1} + \delta V_{DS} \cdot \frac{i - B}{C - B} \quad \text{for } B \leq i \leq C$$

where $\psi_{ij}^0$ is the initial guess, $\psi_{ij}^{-1}$ is the solution obtained from the previous $V_{DS}$, and $B$ and $C$ are the $i$-th column numbers correspond to the two end points of the gate. The graphical representation of this interpolation method is shown in Fig. 3.7. Since no significant change in voltage drop is expected across the drift
regions, which are from the gate (C) to the drain (D), and from the source (A) to gate (B), the initial guesses for these regions are

$$\psi_{ij}^0 = \psi_{ij}^{-1} + \delta V_{DS}, \quad \text{for } C < i < D. \quad 3.55$$

and

$$\psi_{ij}^0 = \psi_{ij}^{-1}, \quad \text{for } A < i < B. \quad 3.56$$

Initial guesses for the carrier concentration $n$ and the temperature $T$ are from the previous two dimensional solution

$$n_{ij}^0 = n_{ij}^{-1} \text{ and } T_{ij}^0 = T_{ij}^{-1}. \quad 3.57$$

because convergence rate is more sensitive to $\psi$ than $n$ and $T$.

The flow chart of the present simulation program is shown in Fig. 3.8.
Drift Velocity vs. Electric Field
($T = 300K$)

$V_{sat} = 1.14e5$ m/s
$u_0 = 0.52 \text{ m}^2/\text{V-s}$

Figure 3.1 Comparison of the overshoot velocity model (OVR) and the exponential model (EXP).
Figure 3.2. Simulated device geometry.

Figure 3.3. Adopted nomenclature for the finite difference method.
Figure 3.4. Flow chart of Gummel's Algorithm.

Figure 3.5. Non-uniform mesh for the MESFET.
Figure 3.6. Five diagonal sparse matrix showing natural ordering by row.

Figure 3.7. Interpolation for the new guess between successive increments in $V_{DS}$. 
Figure 3.8. Flow chart of the present simulation program.
Chapter Four

RESULTS

The Simulation Program

The two-dimensional MESFET simulation program as described in the Chapter Three is implemented in standard FORTRAN. Table A contains the parameter values and the physical dimensions used in the simulation. GaAs MESFETs with and without self-heating effects may both be simulated using the same program with a few minor adjustments. To simulate the device without temperature effects, one can eliminate heat equation which is carried out in the subroutine HEAT at the end of each Gummel's loop. Based on the assumption that no current is injected into substrate, solutions to Poisson's and the continuity equations are limited to the device channel (the shaded region in Fig. 3.2). Without the heat equation, the program does not simulate the substrate portion of the mesh because of the aforementioned assumption. In this case, the simulation time is much faster because fewer mesh points are required.

The first step in verifying the accuracy of the simulation program is to check the five diagonal sparse matrix solver. Stone's implicit method is implemented in two basic subroutines, ODD and EVEN, which correspond to the odd and even loops. The same matrix solver is used by all three decoupled systems of difference equations. The coefficients matrices of Poisson's equation, the continuity equation and the heat equation are generated in subroutines ASMBLP, ASMABLE and ASMBLH respectively. The subroutines ODD, EVEN, ASMBLP and ASMABLE are checked by simulating the potential and electron distributions of a simple resistor (in which the exact analytical solution is known) with Ohmic contacts on two ends and free surfaces on the remaining two sides. The resistor
has the same overall geometry (length \( L = 3.0 \, \mu m \), depth \( A = 0.2 \, \mu m \)), impurity concentration (\( N_D = 6.4 \times 10^{16} \, cm^3 \)) and mobility (\( \mu_0 = 0.52 \, m^2/V\cdot s \)) as the MESFET to be simulated. Only Poisson’s and the continuity equations are solved in this test case. A comparison of the numerical results with the expected resistance for the test case resistor is shown in Fig. 4.1. The good agreement shown indicates that the basic matrix solver is accurate.

Isothermal MESFET

Prior to examining electro-thermal effects on self-heating in the MESFET, the electrical characteristics of an isothermal MESFET were first obtained. The simulation program is setup to simulate the shaded region of the device geometry shown in Fig. 3.2. Thirty-one columns of 0.1 \( \mu m \), and ten rows of 0.02 \( \mu m \) divide the drain to source and the active channel into a uniform mesh.

The simulation program is sensitive to the \( V_{DS} \) step size in the triode region, and thus increments of 0.2V are used between 0V and 1V \( V_{DS} \). Above the saturation voltage, \( V_{DS}^{SAT} \), an incremental change of 0.5V still shows good convergence using the interpolation method shown in Fig. 3.7. With a Schottky barrier height of 0.8eV, \( V_{GS} \) is selected between 0.5V (which is still in the reverse biased region) and -1.0V which is near cut-off. The \( V_{GS} \) step size is not important to convergence because each I-V curve is generated from 0V \( V_{DS} \). The output conductance, \( g_{DS} \), is obtained by averaging \( \Delta J_{DS}/\Delta V_{DS} \) with a \( \Delta V_{DS} \) step size of 0.05V.

Because no experimental data were actually taken for the device simulated, the accuracy of the two dimensional simulation was compared to the three one dimensional analytical models described in Chapter Two in order to verify the overall functionality of the Gummel’s algorithm. The analytical models are
Curtice's model as used in Canfield's work [Canfield, 1990], which does not account for electron velocity saturation, Shur's square law model which accounts for channel length modulation due to velocity saturation, and the complete velocity saturation model. Because both Shur's square law model and the complete velocity saturation model are solved by assuming a two-region piecewise linear velocity-field relationship as shown in Fig. 2.2, this same model is first implemented in the simulation in order to setup a device that closely resembles the approximations used by the analytical models. The series resistances, \( R_S \) and \( R_D \), used in both the square law model and the complete velocity saturation model are approximated by the sheet resistance in the drift regions of the MESFET assuming no depletion region extends beyond the two ends of the gate. Comparisons of the simulated current-voltage relationship to these analytical solutions are shown in Figs. 4.2, 4.3 and 4.4.

The basic Curtice's model used in Canfield's work (Fig. 4.2) grossly overestimates the channel current because it does not take into account the effect of velocity saturation which is a major contributor to current saturation in short channel MESFET's. The square law model shows closer correlation to the simulation results than the previous model, especially at bias points away from cut-off (see Fig. 4.3). Near cut-off of the device, the square law model tends to underestimate the current in the channel. This deviation is due to the assumption that the major contributor to saturation is channel pinched-off, while in an actual device the channel opening remains open due to velocity saturation as discussed in Chapter Two. Based on the same argument, the actual channel length modulation is expected to be less than predicted by \( L_S \) of Eq. 2.5. The lower output conductance ( \( g_{DS0} \), or \( \frac{\partial I_{DS}}{\partial V_{DS}} \) ) observed in Fig. 4.3 supports the argument. The complete velocity saturation model (see Fig. 4.4) provides
close correlation to an actual device near cut-off (where Shur's square law model shows poor correlation), but tends to overestimate when the gate is near forward biased (where Shur's model shows better correlation). Comparison of the output conductance between the complete velocity saturation model and the two dimensional simulation result using the two region velocity-field relationship is shown in Fig. 4.5. The output conductance of the complete velocity saturation model is close to the simulation result considering the numeric accuracy of the small changes in $I_{DS}$ over 0.1V of $V_{DS}$ step size. Because the analytical model assumes the channel opening is only a function of the gate bias when the device is in saturation, the output conductance of the two different drain to source bias, 2V and 3V, are identical. The simulation result of the output conductance at the same two bias points shows the previous assumption used in the complete velocity model is inaccurate. Over the entire simulated bias points, the complete velocity saturation model shows the closest correlation to the simulated result for the geometry of Fig. 3.2. Thus, this analytical model is used in the following sections.

The results discussed in the above section establish the accuracy of the simulation routine without the heat equation. The next step is to replace the two-region piece-wise linear velocity field relationship with more realistic models. The overshoot velocity-field model as described in Eq. 3.12 and shown in Fig. 3.1 is first implemented in the simulation. The I–V curves obtained from the two dimensional simulation using this model is shown in Fig. 4.6. Again, due to the lack of experimental data, the simulated curves are compared to the complete velocity saturation model which showed better overall correlation. With the chosen geometry and doping density, no obvious "oscillation" due to stable negative resistance is observed in the IV curves. However, plots of $g_{DS0}$ versus
$V_{GS}$ and $g_{DS0}$ versus $V_{DS}$, which are Fig. 4.7 and Fig. 4.8, indicate the output conductance does not increase monotonically with $V_{GS}$ or decrease monotonically with $V_{DS}$ as expected for a device not operating in the SNR region. As discussed previously in Chapter 3, this phenomenon is not observed in a real device because current injection into the substrate tends to prevent the formation of SNR. Similar voltage regions of instability were seen in the results of the two—dimension simulation of a GaAs MESFET using the electron temperature model which takes into account the transferred electron effect [Curtice, 1981].

To verify the instability is due to overshoot in the velocity—field model, the exponential model as described in Eq. 3.14 and shown in Fig. 3.1 is implemented in the simulation. The simulated current density (see Fig. 4.9) is lower than expected due to the reduction in the effective low—field mobility ($\mu_{n0}$). Although the exponential model does not provide a good approximation to the actual velocity curve, the I—V curves and output conductance graph (see Fig. 4.9 and 4.10 respectively) show the absence of "oscillation" associated with the overshoot velocity model.

Two dimensional plots of the potential distribution and the electron concentration of two different bias conditions, $V_{DS}$=3.0V, $V_{GS}$=0.5V and −1.0V are shown in Fig. 4.11, 4.12, 4.13 and 4.14. The built—in potential, $V_{BI}$, referenced to the intrinsic level is 0.629eV, and the surface pinning, $V_{BN}$, on the gate is 0.8eV. The x—axis starts from the source contact of the MESFET and ends at the drain contact which is 3μm away. The gate is 1μm in length, and the two drift regions are 1μm each. The y—axis starts at the MESFET's free surface, and ends at the channel/substrate interface, which is 0.2μm away from the surface. Starting from the source contact, the potential is fixed at the built—in potential $V_{BI}$. The voltage drop across the source end of the gate and the source contact is small as
expected, since the only factor contributing to this potential drop is the sheet resistance. The gate contact is fixed at $V_{BI} + V_{GS}$, where $V_{GS}$ is the applied gate voltage. The electron concentration at the source and drain contacts equal to the impurity concentration $N_D$, based on the assumption of ideal Ohmic contacts. The free carrier concentration at the gate is dependent on the gate potential as stated in Eq. 3.39. As expected, a higher $V_{GS}$ (more positive) results in higher potential under the gate (Fig. 4.11) and a smaller depletion region (Fig. 4.12) compared to lower $V_{GS}$ (see Fig. 4.13 and Fig. 4.14). The depletion regions of both cases actually extend beyond the drain end of the gate into the drift region, which is expected for non self-aligned MESFETs. The largest electric field occurs near the device surface within this region. The location of high field region supports the result observed in the Monte Carlo simulation performed by Moglestue [Moglestue, 1981]. Beyond the depletion region to the drain contact, the potential drop is again proportional to the sheet resistance of the channel.

The large variations in both the potential and the carrier distributions demonstrate the power distribution also have large variations both locally within the channel under one bias condition depending on the position in the channel, as well as between different bias conditions. Fig. 4.15, 4.16 and 4.17 show the power density distributions in the channel obtained from the simulation under three bias conditions — non-saturation, saturation and near cut-off. The overshoot velocity model is used in all three cases. When the MESFET is operating in the non-saturation region, the power density is more evenly distributed under the gate. Although the electric field is higher near the device surface and the drain end of the gate (point 1) than the source end (point 2), the localized current density is smaller, thus the location for the peak power density is near the source end. As the device saturates, the power density (Fig. 4.16)
increases and becomes concentrated at the drain end of the gate where the current density is the greatest (point 1). Again, notice the two smaller localized peaks at the drain (point 2) and source (point 3) ends of the gate. The peak at the source no longer dominates the one at the drain because the electric field is higher in the first case due to higher $V_{DS}$. Near cut-off (see Fig. 4.17), the channel depletion region extends close to the channel/substrate interface, the current density is smaller, thus the power density is lower by a factor of ten compared to the previous case.

Non-Isothermal MESFET

As shown in the previous figures, the power distribution along the channel varies strongly as a function of position, the variation of which depends on the bias condition. The large gradient in power density and localization of the heat sources show that the assumption of an uniform channel temperature is erroneous. To study these effects, the heat equation (Eq. 2.13) was included into the simulation as discussed in Chapter Three. The computation time required for simulating non-isothermal conditions is significantly longer than for the case of the isothermal MESFET. Although Poisson’s equation and the current continuity equation are solved only for the channel region because zero conduction is assumed in the substrate, the heat equation has to be solved for both the channel and the substrate. To prevent numerical degeneracy due to long rectangles, the program sets the maximum ratio of the x and y spacings at ten and the ratio of two adjacent x or y spacings to be no more than two. Both contraints affect the simulation time. The simulated substrate depth is selected to be no more than 50µm. This is not unreasonable as the conventional backside mounted MESFETs use substrate thinning and the source contact through via holes, both of which help to extract heat from the channel. Even with the substrate depth limited to
50\mu m the required simulation time is nearly six times longer than the isothermal model.

To setup the test case for a non–isothermal MESFET, several assumptions have to be made. First, based on the assumption that the gate is infinitely wide, the three dimensional heat flow problem is reduced to two dimensions. And, assuming all neighboring devices are infinitely far away, the two artificial boundaries below the source and the drain are treated as adiabatic boundaries ($dT/dn=0$). The third assumption is that both thermal transport mechanisms, which are natural convection and radiation, are negligible. The following proof is to show the validity of this assumption.

Natural convection takes place when heat flows between the MESFET and the air due to temperature difference without the aid of a pump or a fan. Generally the average convective heat transfer coefficient due to natural convection is expressed in the form [Kreith, 1986]

$$h_{cavg} = \frac{k}{P} Nu_{pavg} = \frac{k}{P} C(Gr_p Pr)^n,$$  \hspace{1cm} 4.1

where $k$ is the thermal conductivity of air, $P$ is the characteristic length of the heat source, $Nu_{pavg}$ is the Nusselt number defined by $Gr_p$ and $Pr$, which are the Grashof and Prandtl numbers respectively, and $C$ and $n$ are empirical constants. However, for small devices the classical formula shown above results in large discrepancy with experimental data. An alternative empirical relationship is proposed by Ellison for small devices [Ellison, 1984]

$$h_{cavg} = 2 . 79 \left( \frac{\Delta T}{P} \right)^{0.33} \text{ W/m}^2\text{C},$$  \hspace{1cm} 4.2

For a rectangular horizontal plate heat source the characteristic length $P$ is given by
\[ P = \frac{W L}{2(W + L)} \]

Assuming the heat source is a rectangular horizontal plate of length 4\( \mu \)m and width of 100\( \mu \)m with the heat surface faces upward, at 300K ambient, and a 30°C surface rise, the thermal resistance is given by

\[ R_{\text{conv}} = \frac{1}{h_{\text{cavo}}A} = (652 \text{ W/m}^2\text{C} \times 400\mu \text{m}^2)^{-1} = 3.84 \times 10^6 \text{ K/W}. \]

Heat transfer by radiation may also take place from the MESFET surface to surrounding surfaces. A simple approximation is radiation from MESFET surface to room walls which are at the ambient air temperature. For surface temperatures within 20°C of ambient temperature \( T_A \), and \( T_A \) between 0°C and 100°C, the radiation heat transfer coefficient \( h_r \) can be approximated by [Ellison, 1984]

\[ h_r = 4\sigma T_A^3 = 6.123 \text{ W/m}^2\text{C}, \text{ for } T_A = 300\text{K}, \]

where \( \sigma \) is the Stefan–Boltzmann constant which is equal to 5.670 \times 10^{-8} \text{ W/m}^2\text{K}^4. 

The thermal resistance due to radiation is

\[ R_r = \frac{1}{F A_s h_r} = 1.63 \times 10^{10} \text{ K/W}, \]

for a surface that is small compared to a surface by which it is enclosed, and where \( F \) is the gray body radiation exchange factor equal to the emittance. The emittance for gold is 0.025. The net thermal resistance due to convection and radiation at the MESFET surface is

\[ R_{\text{eq}} = \frac{R_{\text{conv}} R_r}{R_{\text{conv}} + R_r} \approx R_{\text{conv}}. \]

The approximate thermal resistance due to conduction within the MESFET is

\[ R_{\text{cond}} = \frac{1}{\pi k_0} \ln \frac{8 t_{\text{SUB}}}{\pi D} = 447 \text{ K/W}. \]
Since $R_{eq} \gg R_{cond}$, approximating the free surfaces of the MESFET with the adiabatic boundary condition should be adequate.

The above proof shows that neglect of convection and radiation terms in the numerical simulation will not cause significant error in the results. One remaining heat transport mechanism is thermal conduction. Thermal conduction through the device channel and the substrate to the back contact is already discussed in detail in Chapter Three. The back contact is assumed to be an infinite heat sink, where the temperature is fixed at the ambient temperature, $T_A$. The only other factor is thermal conduction through the drain, gate and source contacts. Finding analytical models for the effective thermal resistances for these three contacts is difficult, because thermal conduction coefficient, $h_C$, is strongly dependent on the shape, size and the type of contacts. The extreme case is to assume the drain, source and gate contacts are all infinite heat sinks. Although this assumption will clearly underestimate the channel temperature, it will provide the absolute lower limit. With the aforementioned test conditions, the simulated channel temperature for the MESFET operating in saturation and near forward bias is shown in Fig. 4.18. All three contacts are fixed at ambient temperature of 300K. The peak temperature rise is only 2°C. The location of the peak temperature is at the drain end of the gate near the channel/substrate interface as expected from the power density distribution shown in Fig. 4.16.

A more realistic model than the previous test case is the simulation of a "flip-chip" power MESFET. The "flip-chip", unlike the conventional back-side mounted MESFET, extracts heat through the source contact to a mounted heat sink via a gold post. To simulate the "flip-chip", an infinite heat sink boundary condition is placed on the source contact, while leaving the gate and drain contacts as adiabatic surfaces. The simulated channel temperature of the
MESFET operating in the saturation region and near forward bias is shown in Fig. 4.19. The average thermal resistance, \( \theta_{AVG} \) of the device is

\[
\theta_{AVG} = \frac{T_{AVG} - T_A}{J_{DS} V_{DS}} \, ^\circ C \cdot mm/W,
\]

where \( T_{AVG} \) is the average channel temperature, \( T_A \) is the ambient temperature, \( J_{DS} \) is the drain to source current per unit gate width, and \( V_{DS} \) is the drain to source voltage. The average thermal resistance calculated from the numerical simulation is \( 49^\circ C \cdot mm/W \), where \( T_{AVG} \) is 314K, \( J_{DS} \) is 95mA/mm, and \( V_{DS} \) is 3.0V. The thermal resistance for the "flip-chip" designs found experimentally is typically between 55 and 60 \( ^\circ C \cdot mm/W \) [Wemple, 1982]. The lower thermal resistance obtained from the numerical simulation compared to the experimental data is expected because the actual heat sink and gold post attached to the source contact is not an infinite heat sink. The peak temperature of 319K is located at the drain end of the gate.

An aside should be mentioned concerning the accuracy of experimental results. The three common techniques for determining the MESFET temperature are the Infrared (IR) measurement, Liquid Crystal (LC) measurement, and the electrical measurement [Wemple, 1982]. The temperature measured using the IR technique tends to be lower than the actual channel temperature because the resolution is on the order of 25\( \mu \)m compared to the 1\( \mu \)m gate length. The LC measurement technique, is more accurate, but still limited to a 1\( \mu \)m resolution. The electrical technique, which uses the temperature dependence of the forward biased gate voltage at a fixed gate current, only provides the effective average channel temperature.

The final test case is to treat all three contacts (drain, source and gate) as adiabatic boundaries, and leaving the substrate back contact as an infinite heat
sink. This assumption models a conventional MESFET where the heat is extracted from the back contact using substrate thinning techniques. The current–voltage relationship of the MESFET of Fig. 3.2 with a 20μm substrate depth, and a heat sink through the back contact is shown in Fig. 4.20. Channel self-heating effects are not noticeable when the device is operating near cut–off or in the non–saturation region where the device power dissipation is low. When operating in saturation and with high drain to source current, the temperature in the channel continue to rise until the rate of heat generation is balanced by the rate of heat carried out of the device. This self–heating effect results in a lower saturation velocity and mobility of the carriers as described by Eqs. 3.15 and 3.16, both of which contribute to the decrease in channel current. The thermal conductivity (Eq. 2.14) also decrease with temperature, which further increases the thermal resistivity. The reduction in drain to source current results in negative output conductance (see Fig. 4.21). Similar phenomenon in the DC characteristics is also observed in the two dimensional simulation performed by Ghione [Ghione, 1989]. The space–charge instability region caused by the overshoot velocity is no longer observable as in the case of the isothermal channel, because the electro–thermal effects dominate the g_{DS} profile.

As predicted from the power density plots of the previous section, the temperature distribution in the channel is not uniform. In the triode region, the channel temperature is more evenly distributed under the gate with the peak temperature located near the center of the gate as shown in Fig. 4.22. In the saturation region and near forward bias, a localized heat source occurs at the drain end of the gate where the current density and the electric field are maximum (see Fig. 4.23). When operating near the cut–off region, as shown in Fig. 4.24, the temperature rise is very small because the current density is small.
The substrate temperature profile (Fig. 4.25) is linear from the channel/substrate interface to the back contact. This is expected because the power generation term of the heat equation is assumed to be zero in the substrate based on the assumption of zero current conduction. Because heat is extracted only through the back contact, the channel temperature is dependent on the substrate depth. Three substrate depths of 10\mu m, 20\mu m and 50\mu m are simulated. Shown in Fig. 4.26 shows the one-dimensional temperature distribution profiles from the MESFET surface to the substrate located at the drain end of the gate where the temperature is maximum.

No direct comparison is made between the numerical simulation result and the model proposed by Canfield as discussed in Chapter Two because the former did not take into account of the temperature dependent saturation velocity in the transconductance parameters. Instead, the effective channel temperature equation (Eq. 2.20) is applied to the complete velocity saturation model. The basic analytical model of Eqs. 2.3 and 2.8 of the complete velocity saturation model is modified by the temperature dependent mobility (Eq. 3.15) and saturation velocity (Eq. 3.16), and the average channel temperature based on the half cylindrical model (Eq. 2.20). Comparison of the analytical model and the two-dimensional simulation results is shown in Fig. 4.27. The effective thermal resistance calculated based on the half cylindrical model is 29.8°C-mm/W, and the average channel temperature is 311.7K at V_{DS}=3.0V and V_{GS}=0.5V. The simulated results are 139°C-mm/W, and 352K respectively. Although negative output conductance is also observed in the analytical results using the half-cylindrical model (see Fig. 4.28), the effect of self-heating is significantly less. The large deviation between the two results shows the assumption of an evenly distributed power density in the device channel is erroneous. Both the
increase in peak power density, $P_{T0}$, and the decrease in the effective length of peak power source, $D$, due to localized heat sources cause increase in the overall channel temperature.
<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
<th>units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gate length</td>
<td>LG</td>
<td>1.0</td>
<td>µm</td>
</tr>
<tr>
<td>Active layer thickness</td>
<td>A</td>
<td>0.2</td>
<td>µm</td>
</tr>
<tr>
<td>Donor impurity concentration</td>
<td>ND</td>
<td>6.4E22</td>
<td>m³</td>
</tr>
<tr>
<td>Schottky gate barrier height</td>
<td>V_{BN}</td>
<td>0.8</td>
<td>eV</td>
</tr>
<tr>
<td>Thermal conductivity of GaAs</td>
<td>k</td>
<td>[44(T/300)]^{-1.25}</td>
<td>W/m°C</td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>T₀</td>
<td>300</td>
<td>K</td>
</tr>
<tr>
<td>Low field mobility at 300K</td>
<td>μ₀</td>
<td>0.52</td>
<td>m²/V−s</td>
</tr>
<tr>
<td>Saturation velocity</td>
<td>V_{SAT}</td>
<td>0.64+1.38μₙ−0.82μₙ²</td>
<td>x10⁵ m/s</td>
</tr>
<tr>
<td>Critical electric field</td>
<td>F₉</td>
<td>3.3x10⁵</td>
<td>V/m</td>
</tr>
<tr>
<td>Permittivity in vacuum</td>
<td>ε₀</td>
<td>8.85x10^{-12}</td>
<td>F/m</td>
</tr>
<tr>
<td>Relative permittivity</td>
<td>εᵣ</td>
<td>13.1</td>
<td></td>
</tr>
<tr>
<td>Bandgap energy gap (eV) of GaAs at 300K</td>
<td>E₉</td>
<td>1.42</td>
<td>eV</td>
</tr>
<tr>
<td>Elementry charge</td>
<td>q</td>
<td>1.602x10^{-19}</td>
<td>C</td>
</tr>
<tr>
<td>Intrinsic carrier concentration</td>
<td>Nᵢ</td>
<td>1.79x10^{12}</td>
<td>m³</td>
</tr>
<tr>
<td>Effective density of states in conduction band</td>
<td>N₉</td>
<td>4.3x10^{23}</td>
<td>m³</td>
</tr>
</tbody>
</table>
Resistor Test Case

\[ R_{exp} = \frac{L}{Aqu_0ND} = 0.00281 \text{ V/mA mm}^{-1} \]

\[ R_{sim} = 0.00282 \text{ V/mA mm}^{-1} \]

Figure 4.1 I–V plot of a test case resistor. This test is used to verify the functionality of the matrix solver. The resistance obtained from the 2-D simulation (R_{sim}) is as expected from analytical calculation (R_{exp}).
Figure 4.2 Comparison of the I–V characteristics of the MESFET calculated from Curtice’s model (U0) and from the 2-D simulation result (2Reg) using the two region velocity–field relationship.
Figure 4.3 Comparison of the I–V characteristics of the MESFET calculated from Shur's square law model (SHUR) and from the 2-D simulation (2Reg) using the two region velocity–field relationship.

LG = 1.0μm
ND = 6.4E16 cm⁻³
A = 0.2μm
Vsat = 1.14E5 m/s
u₀ = 0.52 m²/V·s
Figure 4.4 Comparison of the I–V characteristics of the MESFET calculated from the complete velocity saturation model (CVS) and from the 2-D simulation (2Reg) using the two region velocity–field relationship.
Figure 4.5  Comparison of the output conductance obtained from the complete velocity saturation model (CVS) and the 2-D simulation (2Reg) using the two region velocity-field relationship.
Figure 4.6 Comparison of the I–V characteristics of the MESFET calculated from the complete velocity saturation model (CVS) and from the 2-D simulation (OVR) using the overshoot velocity model.
Figure 4.7 Comparison of the output conductance obtained from the complete velocity saturation model (CVS) and the 2-D simulation using the velocity overshoot model (OVR).
Figure 4.8 Output conductance of the MESFET obtained from the 2-D simulation using the velocity overshoot model under three different gate biases. The non-monotonic decrease with respect to Vds shows the effect of NDR due to velocity overshoot.
Figure 4.9 Comparison of the I–V characteristics of the MESFET obtained from the 2-D simulation using the exponential velocity–field relationship (EXP) and the overshoot velocity model (OVR).
Figure 4.10  Comparison of the output conductance obtained from the 2-D simulation using the exponential velocity-field model (EXP) and the overshoot velocity-field model (OVR).
Figure 4.11  Electrostatic potential in the channel of the MESFET under isothermal condition (T=300K). The applied drain and gate voltages (Vds, Vgs) are 3.0V and 0.5V respectively. The built-in potential, Vbi, is 0.629eV. The Schottky barrier height, Vbn, is 0.8eV.
Electron Concentration
Isothermal Channel (Overshoot Model)

Figure 4.12  Electron concentration in the channel of the MESFET under isothermal condition (T=300K).
The applied drain and gate voltages (Vds, Vgs) are 3.0V and 0.5V respectively. The built-in potential, Vbi, is 0.629eV. The Schottky barrier height, Vbn, is 0.8eV.
Figure 4.13  Electrostatic potential in the channel of the MESFET under isothermal condition (T=300K). The applied drain and gate voltages (Vds, Vgs) are 3.0V and -1.0V respectively. The built-in potential, Vbi, is 0.629eV. The Schottky barrier height, Vbn, is 0.8eV.

Diagram:

Electrostatic Potential
Isothermal Channel (Overshoot Model)

DRAIN

SOURCE

GATE

Potential (eV)

Micron (um)

Micron (um)

Potential (eV)

VD = 3.0V
VG = -1.0V
ND = 6.4E16cm^-3
Vsat = 1.14E5m/s
u0 = 0.52m^2/V-s
Figure 4.14  Electron concentration in the channel of the MESFET under isothermal condition (T=300K). The applied drain and gate voltages (Vds, Vgs) are 3.0V and −1.0V respectively. The built-in potential, Vbi, is 0.629eV. The Schottky barrier height, Vbn, is 0.8eV.
Power Density In MESFET Channel
Isothermal Channel (Overshoot Model)

Figure 4.15 Power density in the channel of the MESFET operating in the triode region with the velocity overshoot model. The applied drain and gate voltages are both 0.5V.

VD=0.5V
VG=0.5V
ND=6.4E16cm^-3
Vsat=1.14E5m/s
u0=0.52m^2/V-s
Power Density In MESFET Channel
Isothermal Channel (Overshoot Model)

Figure 4.16 Power density in the channel of the MESFET operating in saturation with the overshoot velocity model. The applied drain and gate voltages are 3.0V and 0.5V respectively.

**Figure 4.16**
- Power density in the channel of the MESFET operating in saturation with the overshoot velocity model. The applied drain and gate voltages are 3.0V and 0.5V respectively.
- **VD=3.0V**
- **VG=0.5V**
- **ND=6.4E16 cm^-3**
- **V_{sat}=1.14E5 m/s**
- **u_0=0.52 m^2/V-s**
Figure 4.17 Power density in the channel of the MESFET operating near cut-off with the overshoot velocity model. The applied drain and gate voltages are 3.0V and -1.0V respectively.
Figure 4.18 Channel temperature of the MESFET operating in saturation and high current density. All contacts are at 300K. The applied drain and gate voltages are 3.0V and 0.5V respectively.
Figure 4.19 Channel temperature of the MESFET operating in saturation and high current density. The infinite heat sink on the source contact is fixed at 300K. The applied drain and gate voltages are 3.0V and 0.5V.

VD = 3.0V
VG = 0.5V
ND = 6.4E16 cm^-3
Figure 4.20 Comparison of the I–V characteristics of the MESFET without self-heating (OVR) and with self-heating (OVRT). Both are simulated using the overshoot velocity model. The substrate depth is 20um. The back contact temperature is 300K.
Figure 4.21 Comparison of the output conductance obtained from the 2-D simulation without self-heating (OVR) and with self-heating (OVRT). Both are simulated using the overshoot velocity model. The substrate depth is 20um. The back contact temperature is 300K.
Figure 4.22 Channel temperature of the MESFET operating in the triode region. The applied drain and gate voltages are both 0.5V. The substrate depth is 20um. The back contact is at 300K.
Figure 4.23 Channel temperature of the MESFET operating in the saturation region. The applied drain and gate voltages are 3.0V and 0.5V respectively. The substrate depth is 20um. The back contact is at 300K.
Figure 4.24 Channel temperature of the MESFET operating near the cut-off region. The applied drain and gate voltages are 3.0V and -1.0V respectively. The substrate depth is 20um. The back contact is at 300K.

VD=3.0V
VG=-1.0V
ND=6.4E16cm^-3
Dsub=20um
Figure 4.25 Channel and substrate temperature distribution of the MESFET operating in the saturation region. The applied drain and gate voltages are 3.0V and 0.5V respectively. The back contact is at 300K.

VD=3.0V  
VG=0.5V  
ND=6.4E16cm^-3  
Dsub=20um
Figure 4.26 Simulated channel and substrate temperature at the drain end of gate for three different substrate depth. The MESFET is operating in the saturation region, with applied drain and gate voltages of 3.0V and 0.5V respectively. The back contact is at 300K.
Figure 4.27 Comparison of the I–V characteristics of the 2-D simulation with self-heating effects (OVRT), without self-heating effects (OVR), and with the complete velocity saturation model with temperature dependent mobility and saturation velocity. The substrate depth is 20um.
Figure 4.28 Comparison of the output conductance obtained from the 2-D simulation using the overshoot velocity model (OVRT) and with the complete velocity saturation model combined with the half cylindrical heat source model (CVST).
Chapter Five

CONCLUSION

The analytical thermal models to date are based on the assumption of uniformly heated channel. As demonstrated from the two-dimensional numerical simulation developed here, this assumption is erroneous and can lead to an underestimated thermal resistance. The simulation provides a detailed description of the power density profile within the active channel under various bias conditions. Except when operating near cut-off and the low current triode region, the power density is far from being uniform within the device. This effect is especially pronounced in saturation and with the gate near forward bias, where localized heat generation is significantly greater than predicted by the power term, $I_{DS}V_{DS}$. The effective heat source is localized at the drain end of the gate where the field and the current density is the largest.

Although the two dimensional numerical simulation program provides a more accurate profile of both the electrical and the thermal characteristics of the device, it does have several limitations. First, the numerical technique used to solve the differential equations have finite error. The difference equations used are themselves approximation to the actual differential equations.

Perhaps more significant than the discretization scheme is the approximation of thermal impedance at the drain, source and gate contacts. Simulation results demonstrated that the effects of heat conductance through these contacts can have significant influence on the overall channel temperature. Another factor which contributed to the limited accuracy of the simulation is the assumption of zero conduction in the channel/substrate interface. In an actual device, substrate conduction will reduce the localized peak current density, thus reducing the peak power density. Since the heat transport equation is dependent
only on power density, reduced peak power density will decrease the channel temperature. To take the substrate current into consideration, one needs to add a finite layer of the substrate into Poisson's equation and the current continuity equations. This improvement should involve the charge balance of EL2 traps in the semi-insulating substrate and any other implanted shallow acceptors, as in buffered devices. Also not considered the present simulation is the lateral effect of the gate width. The simulation assumes the width of the gate is infinitely long such that one may neglect cooling from the third dimension. A three dimensional simulation would be required in order to consider the effect of finite gate width.

The two-dimensional numerical simulation program developed provides more insights to the operation and the electro-thermal effects in GaAs MESFET for power application. The results presented in this thesis may help future development of more accurate analytical thermal models.
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