Design and Simulation of Electrochemical Equivalent Circuit for Extended-gate FET pH Sensor Based on Experimental Value Using LTSPICE XVII

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Design and Simulation of Electrochemical Equivalent Circuit for Extended-gate FET pH Sensor Based on Experimental Value Using LTSPICE XVII

Shaiful Bakhtiar Hashim · Zurita Zulkifli · Sukreen Hana Herman

Abstract

A SPICE model for extended-gate field-effect transistor (EGFET) based pH sensor was developed using standard discrete components. Capacitors and resistors were used to represent the sensing and reference electrodes in the EGFET sensor system and the values of the discrete component were varied to see the output of the transistor. These variations were done to emulate the EGFET sensor output in different pH values. It was found that the experimental transfer and output characteristics of the EGFET were very similar to those from the SPICE simulation. Other than that, the changes of value components in the equivalent circuit did not affect the transfer and output characteristics graph, but the capacitor value produced significant output variation in the simulation. This can be related to the modification on the equivalent circuit was done with additional voltage, $V_{SB}$ (source to bulk) to produce the different $V_T$ values at different pH.

Keywords

Electrochemical method · EGFET · LTSPICE XVII · I-V characteristic

1 Introduction

An electrochemical method capable of translating ion analysis into an existing signal, potential difference, and impedance. This method was commonly used due to its simple operation, good sensitivity, easy miniaturization, and low power consumption. The technique have been used for in situ quantitative analysis and real-time monitoring of environmental parameters and can be divided into three categories, voltammetric, impedimetric, and potentiometric, depending upon the details of the experimental design [1, 2]. Basically, for potentiometric, the electrostatic potentials [volt (V)] are measured and do not involve current in the measurement. While for voltammetric and impedimetric, current measurement is involved and the electrode's potential was held or used as a variable input during measurement.

One example of the electrochemical sensor is ion-sensitive field-effect transistor (ISFET) sensor. The ISFET sensor with a SiO$_2$ insulator as the sensing membrane was reported by Bergveld in 1970 [3]. The basic configuration of ISFET is derived from a metal-oxide semiconductor field-effect transistor (MOSFET), in which the metal gate is substitute by an ion-sensitive membrane with direct contact with a buffer solution [4] but, the ISFET still suffers from several disadvantages, including device instability and poor sensitivity [5]. However, these disadvantages can be overcome by the extended-gate field-effect transistor (EGFET) structure.

EGFET was proposed by Spiegel et al. in 1983 [6]. EGFET structure isolated the FET from the chemical environment, in which a chemically sensitive membrane (or sensing electrode) was deposited at the end of the signal line extending from the FET gate electrode [6]. It offers several advantages, such as light insensitivity, simpler packaging, and flexibility for the shape of the extended gate area [5–7]. EGFET had been applied in an extensive range of applications to detect any substance, especially as biosensors. EGFET is also favorable because it can be characterized using the simple connection and flexibility of the extended gate design [8].

Computer aided design (CAD) tools have made the simulation of semiconductor-based devices possible before going through the complex fabrication process. The CAD will reduce the cost and also design cycle. Simulation Program with Integrated Circuit Emphasis (SPICE) is one the example of CAD tools, which has built-in models for active devices like MOSFETs and Bipolar Junction Transistors (BJTs). The macromodel of ISFET in SPICE was introduced by Martinoia [9]. They came out with the original SPICE-2G and created BIOSPICE that contains a built-in physico-chemical model to
deal with electrochemical devices such as ISFET-based sensors. Other than that, N. L. Mardiah has come out with ISFET macromodel that contributed as a new subcircuit block for LTSPICE IV component library to enable design of ISFET-based sensors or microsystems [10].

ISFET spice model has been widely studied [9], [11–17], but there is still a lack of discussion on the EGFET SPICE model. So, this paper aims to study the equivalent circuit of the electrochemical method with EGFET structure setup simulated using LTSPICE XVII. In addition, based on the theoretical knowledge of the EGFET mechanism, the characteristic and relationship of resistor and capacitor representing sensing electrode (SE) and reference electrode (RE) were studied.

2 Modelling and Simulation Setup

2.1 Electrochemical equivalent circuit

Fig. 1 shows the basic configuration of potentiometric measurement. These basic configurations consist of RE and ion selective electrode (ISE), which convert a particular ionic activity to a specific potential. The potentiometric measurement measures the voltage difference between RE and ISE when both electrodes are dipped in the same buffer solution or electrolyte. The characteristic of ISE controls the ionic activity called response and can be related to the Nernst equation as shown below [18].

\[ E(T) = E^\circ(T) - 2.303 \frac{RT}{nF} \cdot pH \]  
(1)

Where,

- \( E(T) \) = Measured potential mV at temperature T (kelvin)
- \( E^\circ(T) \) = Constant, standard potential mV at temperature T (kelvin)
- 2.303 = Factor to convert ln to log
- \( R \) = Molar gas constant (8.3144 J mol\(^{-1}\) K\(^{-1}\))
- \( F \) = Faraday constant 96485 C mol\(^{-1}\)
- \( T \) = Temperature K (kelvin)

The Nernst equation is a mathematical description of an ideal pH electrode in electrochemistry [19]. It can accurately predict cell potentials only as the equilibrium quotient is expressed in activities. The sensor is considered as a good sensor if the sensitivity value is near to the theoretical Nernstian value of 59.20 mV/pH and the linearity value is near to 1.

Fig. 2 shows the potentiometric equivalent circuit consist of resistors and capacitors. By referring to Fig. 2, resistor (\( R_{REF} \)) and capacitor (\( C_{REF} \)) in parallel represent the RE and resistor (\( R_1 \)) and capacitor (\( C_1 \)) in parallel represent the ISE. In contrast, resistor (\( R_s \)) in series between the two parallel components represent the buffer solution or electrolyte. The value of the potential difference between RE and ISE at different solution buffers is measured by a voltmeter (V).

The capacitor components in this equivalent circuit can be described with Helmholtz double layer, which represents the accumulation of electrical charges present at the boundary of an electrode and electrolyte when they are in contact with each other as in Fig. 1. The arrangement of positive and negative charge at the surface of electrode leading to the capacitive behavior of charge storage [20]. While, the resistor's role is to oppose the electrical current through it. This is called the resistance of electricity, which is measured in the ohm unit. The capacitance (C) and resistance (R) equation are shown below:

\[ C = \frac{q}{V} \]  
(2)

\[ R = \frac{V}{I} \]  
(3)
Where,

\( C = \text{capacitance of capacitor, Farads (F)} \)
\( q \) = charge stored, Coulombs (C)
\( V = \text{voltage, Volts (V)} \)
\( R = \text{resistance, Ohms (Ω)} \)
\( I = \text{current, Amperes (A)} \)

### 2.2 EGFET setup equivalent circuit

Fig. 3 shows the experimental EGFET measurement setup. The RE was connected to a Semiconductor Device Analyzer (SDA) Keysight B1500A, while the SE was connected to the gate of a commercialized MOSFET CD4007 as the extended gate sensing electrode. This MOSFET is well documented in terms of width and length in the SPICE model, and the connectivity of this MOSFET also versatile. The transfer and output characteristic was obtained from this measurement setup.

Fig. 4 shows the internal schematic circuit of CD4007 MOSFET. The CD4007 consist of 3 pairs inverter with pin 14 as P-type metal oxide semiconductor (PMOS) and pin 7 N-type metal oxide semiconductor (NMOS). This inverter shares a common pin gate (6, 7 and 10). In this measurement, pin 6, 7 and 8 were used for measurement. Other pins (3, 4, 5, 10, 9 and 12) also can be used for measurement setup. The EGFET equivalent circuit as shown in Fig. 5 has been constructed by considering the potentiometric equivalent circuit (Fig. 2). The difference between Fig. 2 and Fig. 5, Fig. 5 has additional NMOS MOSFET representing CD4007 that gate connected to sensing capacitor (C1) and resistor (R1) while reference voltage, \( V_{\text{REF}} \) connected to reference capacitor (\( C_{\text{REF}} \)) and resistor (\( R_{\text{REF}} \)).

Fig. 6 shows the basic reaction on metal oxide surface producing surface potential at (a) neutral, (b) acidic, and (c) alkaline conditions. As shown in Fig. 6, at the surface of metal oxide it has a hydroxyl group [21] and these hydroxyl groups are capable of interacting with pH potential determining ions (PDI) which is hydrogen ions (in acidic solution) and hydroxide ions (in basic solution). Depending on the type of PDI that is dominant in the solution, the surface of the sensing membrane will be either more positively or more negatively charged. This positively and negatively charged can be represented by the capacitor C1 in EGFET equivalent circuit (Fig. 5). The change of ion is detected based on the changes in capacitance. The amount of charge that can be adsorbed on the capacitor shall be determined by the capacitance. In EGFET equivalent circuit, resistor \( R_{\text{REF}} \) and R1 act as the charge transfer resistance and \( R_{S} \) is the solution resistance.
3 Analytical Modelling Approach

3.1 Simulation for EGFET equivalent circuit
In this simulation part, LTSPICE XVII was used to simulate the EGFET equivalent circuit and studied each component’s characteristics and relationship toward the current voltage (I-V) characteristic. Before running the simulation, CD4007 MOSFET was modelled by setting up the parameters of the MOSFET such as width (W), length (L), transconductance (K), lambda (λ) and threshold voltage (V_T) as shown in Table 1.

Fig. 7 and 8 show the experimental output and transfer characteristics of CD4007 MOSFET, respectively measured using SDA. The value of V_DS was varied from 1 to 3 V and V_GS was fixed at 2V for output characteristic. While for transfer characteristic, V_GS was varied from 1 to 3 V and V_DS was set at 100 mV.

As shown in Fig. 7, there are three state regions: triode, linear, and active. These regions represent by the given formula as shown in equations (4), (5), and (6) as follows:

\[ I_D = \mu_n C_{ox} \frac{W}{L} (V_{GS} - V_t) V_{DS} ; \]
Triode region
\[ I_D = \mu_n C_{ox} \frac{W}{L} (V_{GS} - V_t) V_{DS} - \frac{V_{DS}^2}{2} \]
Linear region
\[ I_D = \frac{1}{2} \mu_n C_{ox} \frac{W}{L} (V_{GS} - V_t)^2 ; \]
Active region
\[ K = \mu_n C_{ox} ; \text{Transconductance} \]

Where \( I_D \) is drain current, \( \mu_n \) is the mobility, \( C_{ox} \) is the oxide capacitor, W is width, L is length, V_GS is gate-source voltage, V_DS is drain-source voltage, and V_T is the threshold voltage. Three formulas represent three conditions from Fig. 8, cut-off region, linear region and saturation region.

![Fig. 7 Output characteristic (I_D versus V_DS) of CD4007UBE using Semiconductor Analyzer](image)

![Fig. 8 Transfer characteristic (I_D versus V_GS) of CD4007UBE using Semiconductor Analyzer](image)

### Table 1
MOSFET PARAMETERS FOR LTSPICE SIMULATION

| MOSFET Parameter       | Value     |
|------------------------|-----------|
| Width (W)              | 170 μm    |
| Length (L)             | 10 μm     |
| Transconductance (K)   | 74.33x10^{-6} S |
| Lambda (λ)             | 0.01      |
| Threshold Voltage (V_T)| 1.1 V     |

Formula (7) and (9) describe the condition, respectively. The cut-off region where \( V_T \) is less than or equal VGS, while for a linear region, V_GS greater than V_T. As shown in Fig. 9, the value of V_T was around 1.1 V, and at V_GS 3 V the value of drain current, I_D was around 234 μA. The value of W and L was assumed and fixed to 170 μm and 10 μm, respectively. The value of λ was also assumed to be 0.01.

\[ I_D = 0; V_{GS} \leq V_T ; \]
Cut Off
\[ I_D = K \frac{W}{L} [(V_{GS} - V_t) V_{DS} - \frac{V_{DS}^2}{2}] (1 + \lambda V_{DS}) ; \]
Linear region
\[ V_{GS} > V_T, V_{DS} \leq V_{GS} - V_T ; \]
\[ I_D = K \frac{W}{L} (V_{GS} - V_T)^2 (1 + \lambda V_{DS}); \]

\[ V_{GS} > V_T \quad V_{DS} > V_{GS} - V_T; \]

Saturation region \hspace{1cm} (9)

By referring to (7), the value of \( V_{GS} \) (3 V) is greater than \( V_T \) (1.1 V), and in the other condition, the value of \( V_{GS} - V_T \) (3-1.1) is greater than \( V_{DS} \) (100 mV). Based on these conditions, the value of transconductance, \( K \) can be calculated using the formula and found to be 74.33μS. Therefore, all these parameters \( W \) (170 μm), \( L \) (10 μm), \( K \) (74.33 μS), \( V_T \) (1.1 V) and Lambda (0.01) were set in LTSPICE simulation as shown in Fig. 9.

In this paper, the simulation was carried out for \( I_D \) versus \( V_{GS} \) at fixed \( V_{GS} \) at 3V, \( I_D \) versus \( V_{DS} \) for \( V_{GS} \) fixed at 2V, with different capacitor and resistor values.

Other than that, the output current for variation of equivalent circuit, input and output characteristic at different pH levels, and input and output characteristic for different \( V_{REF} \) also were studied.

4 Results and Discussion

4.1 Graph analysis on simulation and experimental

For this part of a simulation, Fig. 10 and 11 are the \( I_D \) versus \( V_{GS} \) and \( I_D \) versus \( V_{DS} \) for EGFET equivalent circuit parameters, as shown in Fig. 9. Fig. 10 shows the output characteristic measured using SDA shows the value of \( I_d \) at 2 V \( V_{DS} \) is at 307 μA, but from the simulation result, the \( I_d \) at 2 V is greater than 500 μA. The value of \( I_d \) that closed to 307 μA when the \( V_{GS} \) value at 1.8 V. So, it can be said that the simulation part and the actual are set to be the same condition. Even though \( I_D \) values are slightly different between simulation and using SDA, but this value is acceptable. Fig. 11 shows that \( V_{GS} \) at 3 V exhibited the value of \( I_D \) at 234.002 μA, which is similar to the transfer characteristic of CD4007UBE using SDA.

4.2 Analysis on the reference and sensing electrode equivalent circuit

In this part of simulation, each component \( C_{REF}, R_{REF}, R2, C1 \) and \( R1 \) was varied from low to a high value to observe the output changes in \( I_D \) versus \( V_{GS} \) graph. The resistor was varied from 10 Ω to 1000 kΩ, while for capacitor was varied from 0.1 μF to 4700 μF.

Table II shows the output of the current \( I_d \) when the value of the component in EGFET equivalent circuit was changed. The simulation result showed no changes on the \( I_d \) current for the different values of \( R \) and \( C \). Due to no changes for each component, \( R2 \) has been replaced with the voltage source, \( V_{R2} \) by assuming the voltage source act as potential differences between the two electrodes as shown in Fig. 12.
As shown in Table II, as the value of $V_{R2}$ increases, the $I_d$ also increases. It shows that the potential difference at $V_{R2}$ may result in different output values. This situation obeys the Nascimento et al. [22], in which there are potential differences between RE and SE. That the ions in the solution are eventually attached to the sensor's surface due to their affinity with these ions. Consequently, the value of voltage will change according to a different solution and sensing film, then the result will lead to an extra variable potential $\Delta V$ between the bulk solution and the surface of the film.

| $V_{ref}$ | $V_{DS}$ | $C_{ref}$ | $R_{ref}$ | $R_2$ | $C_1$ | $R_1$ | $I_d$ | $V_{Rs}$ |
|----------|----------|-----------|----------|--------|--------|--------|-------|---------|
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |

**Fig. 13** (a)-(d) shows different configurations of the EGFET equivalent circuit to observe if there are any changes in the $I_d$ versus $V_{GS}$ graph. Fig. 13 (a) basically same as Fig. 8, Fig. 13 (b) shows that all capacitors and resistor have been removed, while Fig. 13 (d) only capacitor and resistor for reference electrode part and Fig. 13 (c) capacitor and resistor for reference part as well as resistor $R_2$.

**Table II**

**SUMMARIZE OUTPUT FOR EACH COMPONENTS**

| $V_{ref}$ | $V_{DS}$ | $C_{ref}$ | $R_{ref}$ | $R_2$ | $C_1$ | $R_1$ | $I_d$ |
|----------|----------|-----------|----------|--------|--------|--------|-------|
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |

**Table III**

**SUMMARIZE OUTPUT FOR DIFFERENT $V_{R2}$**

| $V_{ref}$ | $V_{DS}$ | $C_{ref}$ | $R_{ref}$ | $R_2$ | $C_1$ | $R_1$ | $I_d$ |
|----------|----------|-----------|----------|--------|--------|--------|-------|
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |
| 3        | 0.1μ     | 10Ω       | 100      | 0.1μ   | 10Ω    | 10Ω    | 234.002μA |

**Fig. 13** (a)-(d) Different types of equivalent circuit
The simulation result shows the output for all equivalent circuits exhibited the same graph and where the value of $I_D$ equals to 234.002 $\mu$A. However, when a capacitor was added in series with $R_2$ as shown in Fig. 14, shows 209 fA. The output graph was shown in Fig. 15.

The output was obtained when the $V_T$ is set to 1.1V. The result shows a very small output current that is equivalent to 209 fA and was not affected by the $V_{GS}$ changes. However, when the $V_T$ was changed to 0V, the output characteristic shows an exponential output curve as shown in Fig. 16, meaning that the $I_D$ was slowly increased with the increase of $V_{GS}$ value (0-3V).

4.3 Comparison of SPICE simulation and experimental results

Fig. 17 and 18 show the output and input characteristics measured by SDA with EGFET setup at different pH values (pH 2, 4, 6, 7, 8, 10 and 12) respectively. The output characteristic shows that the drain current, $I_D$, was decreasing as the pH value increases and it shows that low pH yields high $I_D$. Fig. 19 shows $I_D$ versus $V_{DS}$ graph at different $V_{REF}$ values using LTSPICE simulation by using an equivalent circuit in Fig. 9. The graph shows similar output pattern as Fig. 17, where the higher the pH value, the lower the drain current. For Fig. 19, it shows that pH 12 exhibited drain current of around 500 $\mu$A and for pH 2 shows 50 $\mu$A. The graph also shows that the $I_D$ and $V_D$ is proportional and linear until $I_D$ is saturated and produced a constant value for each pH value.
Fig. 20 shows $I_D$ versus $V_{GS}$ at different $V_{DS}$ values using LTSPICE simulation, the $I_D$ has changed with $V_{DS}$ value, but the output started at the same $V_T$ for all values of pH value. The characteristic is not the same as what was obtained from the experimental work. Thus, a modification of the equivalent circuit is needed.

Fig. 21 shows the modified equivalent circuit with additional voltage, $V_{SB}$ (source to bulk). The Body effect refers to the changes of the transistor threshold voltage resulting from a voltage difference between the transistor source and body. Because the voltage difference between the source and body affects the $V_T$, the body can be considered a second gate that helps determine how the transistor turns on and off [23].

By varying the $V_{SB}$ and fixed the value of other components, it shows the different values of $I_D$ at different values of $V_T$ were obtained as shown in Fig. 22. For example, at lower pH 2, the value of $V_T$ was around 5.5 V, and for pH 12 the value of $V_T$ was around 1.15 V which is a similar pattern to the experimental results.

**5 Conclusion**

In this paper, the EGFET equivalent circuit and different types of the equivalent circuit have been successfully simulated by using LTSPICE XVII using discrete components. The success of modeling and simulation can contribute to the prediction of the output current based on different pH level. From the results, the simulation graph for transfer characteristics showed very similar pattern with SDA but for the output characteristic graph, there was a slight difference in terms of the value of drain saturation current. Other than that, we found the resistor and capacitor value in the equivalent circuit did not affect the transfer and output characteristics, but the parameter inside MOSFET such as width, length, transconductance and threshold voltage play an important role. The modified equivalent circuit with additional voltage, $V_{SB}$ (source to bulk) produces the different $V_T$ values at different pH values which is similar to the experimental results.

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