Determination of Flat band and Drain Voltage for Maximum Sensitivity and Linearity of Electrolyte sulator Interface Si3N4 Field Effect Sensor to H+ I Concentration Based on PSpice Macro Model

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Abstract: - Integration of ISFET sensor with signal processing circuits has made it easier, thus enabling simpler and portable application, even potential on-site screening is possible with the recent advances of electrochemical sensors and silicon technology. ISFET sensor fabricated with CMOS technology benefits from low cost production, low power and miniaturization enabling for micro system. ISFET sensor is fundamentally a MOSFET with a gate structure comprising of a reference electrode and insulator. The ion concentration of electrolyte which completes the gate-source circuit, affects the gate potential to produce threshold voltage. It serves at the front end of the instrumentation system, with a critical role to interface between the electronic signals and measured signals. OrCAD PSpice facilitates the design and testing of circuitry before the costly fabrication, with a drag-n-drop sub-circuit block library of macro models. However, even with its current popularity, macro model for ISFET devices is not found. The paper proposes a macro modeling approach for the physical-chemical behavioral model of ISFET, to contribute to a new sub-circuit block for PSpice, to allow characterization and parameterization of such devices to be simulated. Its functional quality is ascertained by comparing its drain current characteristic against that generated from source code from previous work, with ±8% discrepancy in sensitivity for pH [4 7 10]. Then, it is used to design parameters for a Si_3N_4 FET sensitive to H+ ion, for operation characteristic to be as linear and sensitive as possible. The drain and flat band voltage optimal for this requirement are found to be 0.1volt and 1.5volt respectively. In the case of drain voltage, it is found that smaller voltage produces faster and more sensitive response. Higher drain current and lower cut-off voltage yields higher sensitivity. At the optimal drain voltage of 0.1volt, a sensitivity of 54.79mV/pH is reported. In the case of Vbias, Vbias of 1.5volt is preferred to 1.0volt for linear change in drain current to pH value.

Key-Words: - ISFET, H+ Ion, pH, PSpice, OrCAD, Macro-model.

I. INTRODUCTION

Measuring and sensing chemical environment is one of the basic functions of a micro system which can be used in many applications such as pharmaceuticals, food processing and healthcare to validate process industry [1][2]. Mathematical models play an important role in the analysis of the chemical system in order to know the structure of the sensor [3]. The sensory behavior of the sensor has to be modeled in order to interact between hardware and software of the instrumentation system [4].

Ion selective field effect transistor (ISFET) is a solid state micro sensor that was initially developed for detecting H+ ion, which is then extended to detect other ions such as potassium, sodium. It has proven to be useful in the field of biomedical engineering, agriculture, environment, food industry and so on [5]. ISFET sensor serves at the front end of instruments in data acquisition system, interfacing between the electronic signals and measured signals in different forms. Its functional quality is critical to the instrumentation system. If it is poor, the quality of the transformed electronic signals will not improve, even with the most sophisticated signal processing. Previous works has found research on H+ ISFET for application as the front end sensor in automated screening or specimen analysis. An example being a Stow-Severinghus potentiometric cell H+ ISFET for sensing blood dissolved CO_2 based on permeation through membrane [6]. Another example is the use of electrochemical potentiometric cell H+ ISFET to detect blood and urea acidity, working on H+ ion complexation in membranes [6][7]. Recent advances in the electrochemical sensor and silicon technology has made it easier for ISFET sensor to integrate with signal processing, thus enabling simple and portable measurement, even potential on-site screening.

Low cost production, low power and miniaturization enabling for micro system with monolithic integration are just a few of the many benefits of ISFET sensors fabricated with Complementary Metal Oxide Semiconductor (CMOS) technology, which sensors from discrete electronic components could not contend. ISFET has a physical structure similar to MOSFET, except for the metal gate being replaced by a cascade of reference electrode, electrolyte and chemically sensitive insulator. In the case of aqueous pH, the principle of detection by electrochemical means is anchored on the sensitivity to the H+ ion, which silicon nitride (Si_3N_4) membrane is found stable and hence suitable [8].

OrCAD PSpice is a circuit analysis program that allows analogue only circuit design to be created, simulated and tested, while OrCAD Capture allows schematic of the circuit design to be captured, which is then used to generate input format suitable for PSpice or other printed circuit board (PCB) layout design programs. The former facilitates design and fine-tuning of circuitry before the costly

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fabrication, while the latter produce the schematic layout necessary for fabrication. Built into the software are macro models, a library of theoretical models, related closest to our work are the macro model of MOSFET and its derivatives. However, even with its growing popularity, macro model for the H+ ISFET device is not available.
This paper proposes development of a new macro model to describe the physical-chemical behavioral model of ISFET, to add to the sub-circuit block library of PSpice. This new PSpice macro model contributes in that it can be extracted, exported and used by other PSpice-based simulation tools. This then allows the parameterization and characterization of such devices to be simulated before the fabrication, to save cost. Firstly, derivation of the mathematical model of ISFET is presented. This is then followed by explanation on the method to build its macro model in PSpice. Having verified its function against previous work, the newly generated macro model is then used to determine the optimal value for drain voltage and Vbias for adequately sensitive and linear characteristic of the H+ ion sensitive FET sensor.

2 MACRO MODELING OF H+ ISFET

The surface of the n-channel ISFET structure in Fig. 1 is made of an insulator layer Si_3N_4 exposed to an aqueous electrolyte solution, with a p-type semiconductor and a Si_3N_4 insulator in it. The gate consists of a reference electrode and dielectric, which flows the electrolyte. Its potential depends on the ionic concentration of electrolyte and affects the threshold voltage of transistor. The ionic concentration of electrolyte generates an electrostatic control on the drain-source current. Hence, change in it incurs change in the drain current, which is then compensated by adjusting the reference electrode potential, or gate voltage, since normal operation of ISFET is in the constant drain current mode. As such, the sensitivity of ISFET is expressed as change in gate voltage per decade of ion concentration [10].

Representation of the H+ ISFET entails two mutually independent models. The electrochemical model describes the electrolyte insulator interface while the electronic model describes the structure of ISFET Construction of the electrochemical model is first introduced.
With reference to the charge neutrality in the structure of Fig. 1 and assuming that σ_s is very small relative to σ_o and σ_d , in fact constant for pH,

$$\sigma_o + \sigma_d = 0 \qquad (1)$$

where σ_o, σ_d, σ_s are charge densities at the electrolyte insulator interface and diffuse layer in the semiconductor [9,11].

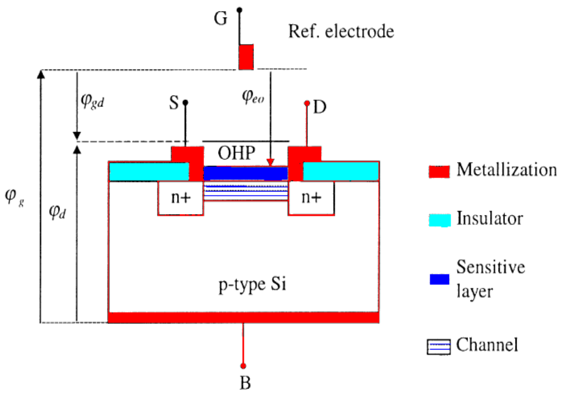

Fig. 1: An n-channel ISFET structure.

Based on H+ specific site binding theory and electrical double layer theory[12] σ_o and σ_d are defined as follows,

$$\sigma_d = \sqrt{8\varepsilon_w kT c_{bulk}} \sinh\left(\frac{\varphi_{gd}}{2V_T}\right) \qquad (2)$$

$$\sigma_o = qN_{Sil}\left(\frac{H_b^2 \exp\left(-2\frac{\varphi_{eo}}{V_T}\right) - K_A K_B}{H_b^2 \exp\left(-2\frac{\varphi_{eo}}{V_T}\right) + K_A H_b^2 \exp\left(\frac{\varphi_{eo}}{V_T}\right) + K_A K_B}\right) + qN_{Nit}\left(\frac{H_b^2 \exp\left(\frac{\varphi_{eo}}{V_T}\right)}{H_b^2 \exp\left(\frac{\varphi_{eo}}{V_T}\right) + K_N}\right) \qquad (3)$$

where ε_W and c_{bulk} is the permittivity and ion concentration of electrolyte, N_{Sil} and N_{Nit}; φ_{gd} is the potential across the diffusion layer; V_T is the thermal voltage; K_A, K_B, K_N are the binding site dissociation constants; H_b is the proton concentration of the bulk electrolyte; φ_{eo} is potential of the electrolyte insulator interface.

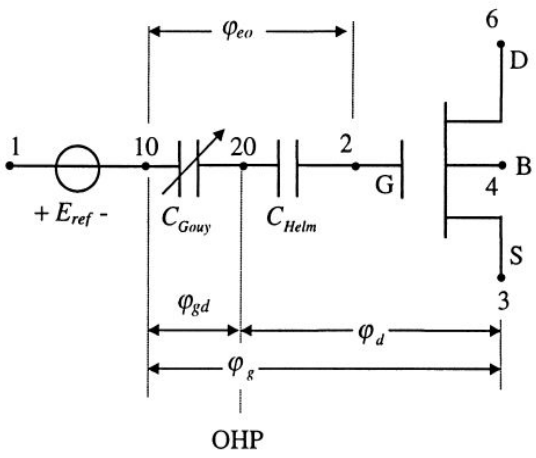

Fig. 2: Analogous electrical model to the electrochemical model for ISFET structure.

With the above, an analogous electrical model to the electrochemical model in Fig. 2 can be developed. Capacitance in series, C_{Gouy} of diffuse layer and C_{Helm} of Helmholtz layer can be substituted by the equivalent capacitor C_{eq} in the macro model as follows,

$$C_{eq} = \frac{C_{Gouy} C_{Helm}}{C_{Gouy} + C_{Helm}} \qquad (4)$$

$$C_{Helm} = \frac{\varepsilon_{IHP}\varepsilon_{OHP}}{\varepsilon_{OHP} d_{IHP} + \varepsilon_{IHP} d_{OHP}} WL \qquad (5)$$

$$C_{Gouy}=\frac{\partial\sigma_d}{\partial\varphi_{gd}}=\frac{\partial}{\partial\varphi_{gd}}\left[\sqrt{8\varepsilon_w kT c_{bulk}}\,\sinh\left(\frac{\varphi_{gd}}{2V_T}\right)\right]=\frac{\sqrt{8\varepsilon_w kT c_{bulk}}}{2V_T} \qquad (6)$$

where W and L are the channel width and length of ISFET; ε_{IHP} and ε_{OHP} are the inner and outer Helmholtz plane permittivity; d_{IHP} and d_{OHP} are the insulator non-hydrated ion and the insulator hydrated ion distance accordingly. The Hemholtz layer is directly proportional to the length and width of the channel. For the Gouy–Chapman capacitance, the assumption $\varphi gd \ll 2VT$ is made.

By substituting (5) and (6) into (3), the charge densities at the electrolyte insulator interface becomes,

$$\sigma_o = \left[qN_{Sil} f_a(\varphi_{eo}, pH) + qN_{Nit}(\varphi_{eo}, pH)\right] \qquad (7)$$

which gives rise to the potential of the electrolyte insulator interface,

$$\varphi_{eo} = \frac{q}{C_{eq}}\left[N_{Sil} f_a(\varphi_{eo}, pH) + N_{Nit}(\varphi_{eo}, pH)\right] \qquad (8)$$

This equation corresponds to a non-linear voltage controlled source, which depends on both of pH and φ_{eo} [9]. Together with (5), the electrochemical behavior of ISFET is translated into the analogous electrical model in Fig. 2. It can be used as an electronic device for designing pH sensors or any ISFET-based micro-systems. The pH-independent source is designated as a chemical input signal, modeled by an independent voltage source, connected to a dummy resistor. The macro model uses this voltage to simulate the pH value. In addition, it also acts as an electrochemical source that controls φ_{eo} in (8).

The H+ ISFET macro model is built, with existing MOSFET macro model as its starting structure, which then refined to a behavioral macro model for ISFET. Hence, the description of ISFET macro model follows that of MOSFET. The physical-chemical behavior of ISFET is built into the library of drag-n-drop sub-circuit blocks of PSpice with Orcad Capture, a schematic entry program. Fig. 3 shows the ISFET capture symbol, with outer connection 1 for drain, 2 for reference electrode, 3 for source, 4 for bulk and 5 for input, such as the chemical input signal representing pH in our work.

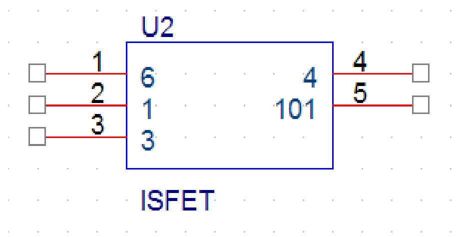

Fig. 3: ISFET CAPTURE symbol

3 RESULTS AND DISCUSSION

Fig. 4 shows the flow chart on how the new library for ISFET is created on PSpice. Fig. 5 shows simulation with the new H+ ISFET sub-circuit block. Before this, characteristic of its drain current is measured against that of its equivalent mathematical model [9]. At the same Vd and Vbias, it is found that both responses are similar, with discrepancy of ±8% in sensitivity for pH [4 7 10]. After the simulation is set up, the PSpice Schematic generates a circuit file set, containing circuit netlist and analysis command, which is read by PSpice A/D for simulation.

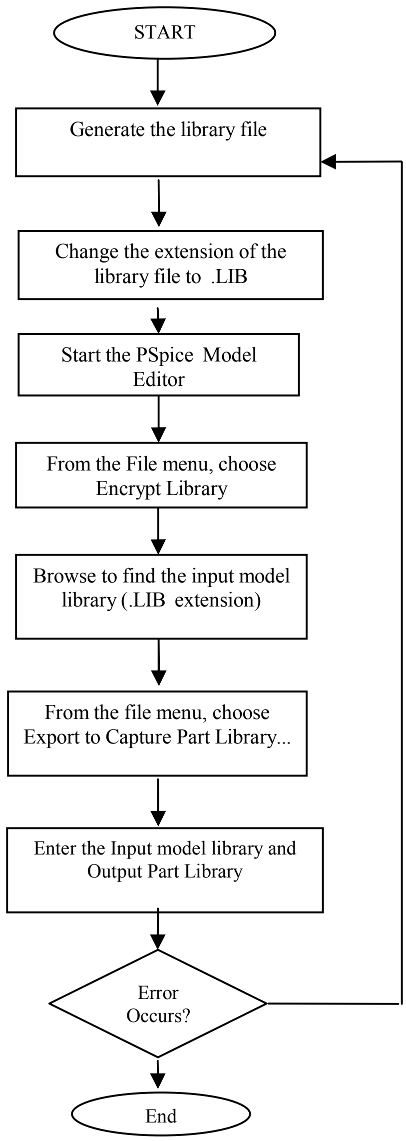

Figure 4: Flowchart for creating capture symbol (ORCAD CAPTURE) and new library part for PSPICE

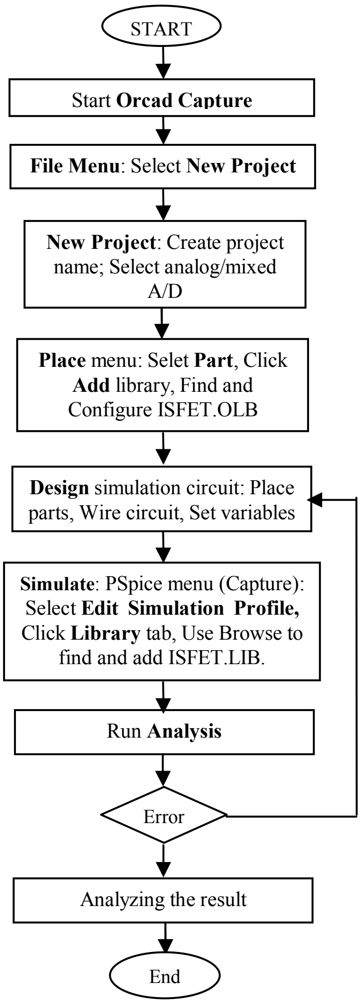

Fig.5 : Simulation of H+ ISFET with ORCAD CAPTURE

3.1 SELECTING OPTIMAL Vd

Firstly, the characteristics of drain current with voltage variables, Vbias and Vd is examined. This is to derive the change in the threshold voltage to pH, so that optimal Vd for high sensitivity can be determined.

Fig. 5a, 5b and 5c shows the variation in drain current (Id) with simulated input to H+ ISFET (Vbias) at drain voltage (Vd) of 1.0volt. As Vbias increases, Id follows a first order response and then saturates, for all pH values at the electrolyte insulator interface. At saturation, the input voltage bears no effect on the output current. Drain current reads higher with lower pH value, at constant Vd and Vbias, owing to higher ionic concentration.

Similar response with different degree of damping and values is obtained when Vd is increased to 0.5volt and 1.0volt. Response reacts faster and less sluggish with smaller Vd. Over the same range of Vbias, the smaller is the Vd, the wider is the span of Id. This implies higher sensitivity in reacting to changes in Vbias for smaller Vd. For the same reason, Id reads higher for the same Vbias, with smaller Vd, at constant pH.

From Fig. 5a ,5b and 5c at constant Vd, different pH is found to have different cut-off voltage, the higher the pH value, the cut-off voltage is higher. As Vd increases, the cut-off voltage is also higher.

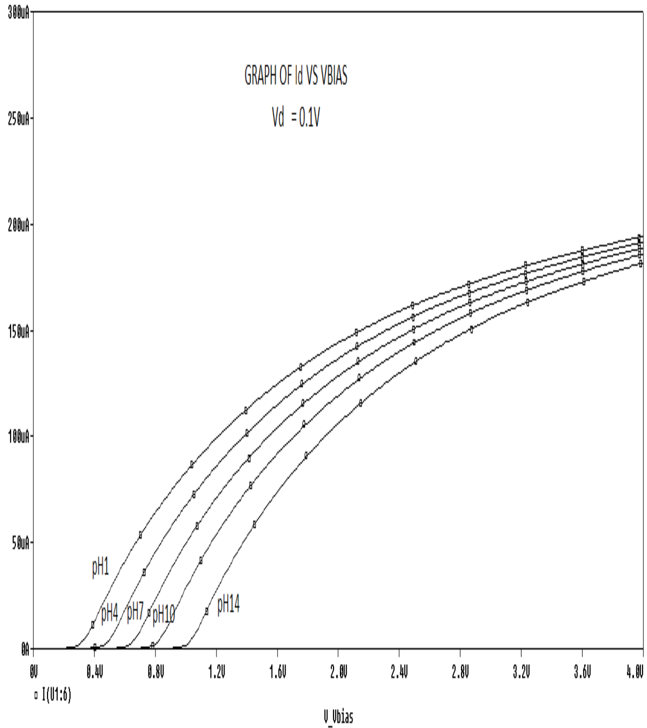

Fig. 5a: Variation of Id with Vbias at Vd of 0.1V

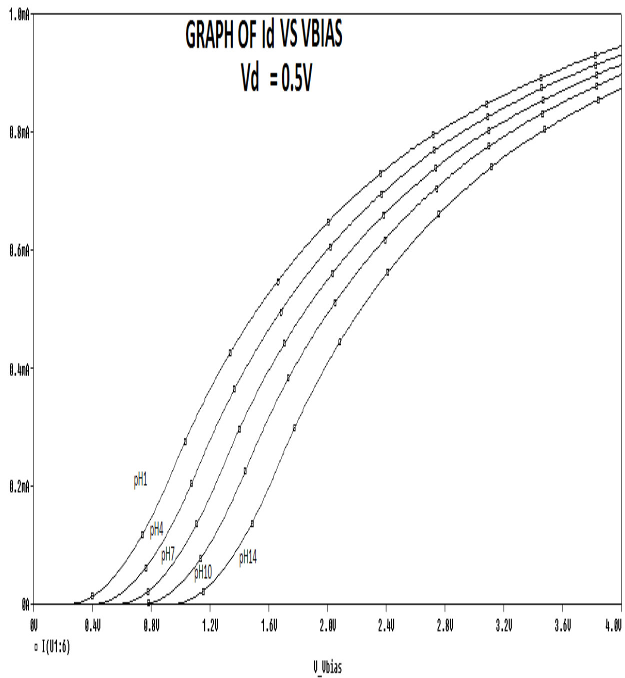

Fig. 5b: Variation of Id with Vbias at Vd of 0.5V

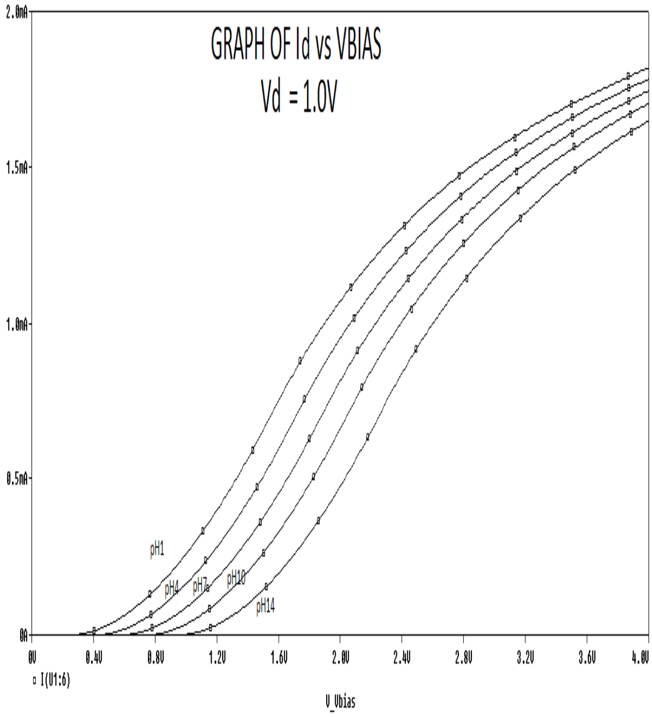

Fig. 5c: Variation of Id with Vbias at Vd of 1.0V

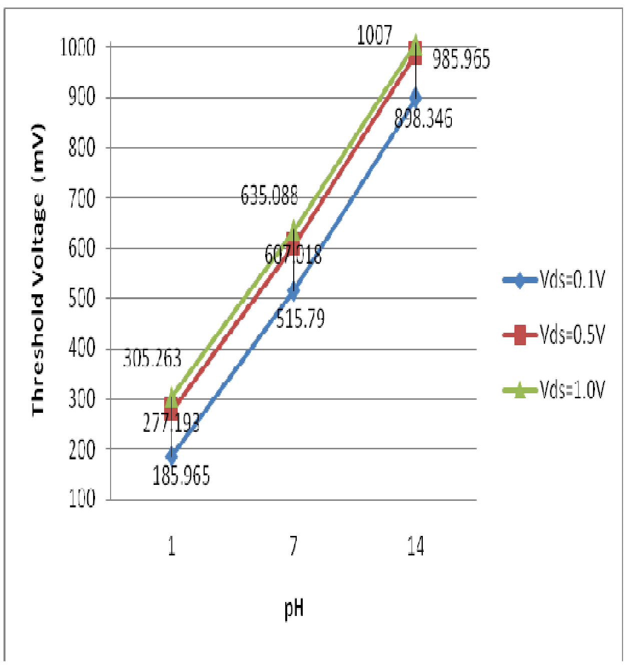

Fig. 6: Characterization of pH against threshold voltage

An important characteristic to consider in selecting Vd to describe the behavior of ISFET is sensitivity. Fig. 6 relates the threshold voltage of H+ ISFET, derived from the responses of Id, shown in Fig. 5a,5b and 5c to pH at the electrolyte insulator interface. Value of pH [1 7 14] is used to indicate the states of electrolyte [Acidic Neutral Alkaline]. At constant pH, the threshold voltage is found to increase with Vd.

TABLE 1
SENSITIVITY OF H+ ISFET FOR DIFFERENT VALUES OF Vd

	Sensitivity (mV/pH)
Vd = 0.1V	54.79
Vd = 0.5V	54.52
Vd = 1.0V	53.98

Table 1 shows the sensitivity derived from the gradient of graphs in Fig. 6. It can be observed that sensitivity increases with decrease in Vd. At Vd of 0.1volt, sensitivity is highest, at 54.79 mV/pH, which explains it being selected as the optimal parameter for H+ ISFET.

3.2 SELECTION OF V_{bias} (FLAT BAND VOLTAGE)

Two important characteristics to consider in selecting Vbias to describe the behavior of ISFET are sensitivity and linearity. Sensitivity is the

Firstly, sensitivity in selecting Vbias is considered. Fig. 7a, 7b, 7c and 7d display the variations in Id with Vph, at Vbias of 0.3volt, 1.0volt, 1.5volt and 2.5volt. Fig 7b and 7c shows that the Id versus Vph having the most linear behaviour. Similar but less linear graph is observed with Vbias of 0.3volt and 2.5volt. In comparison, Vbias of 1.0volt is found to produce a higher sensitivity of 5.04µA/V (see Fig. 7b) compared to that by Vbias of 1.5volt, with a sensitivity of 3.38µA/V. The sensitivity decreases as Vbias increases.

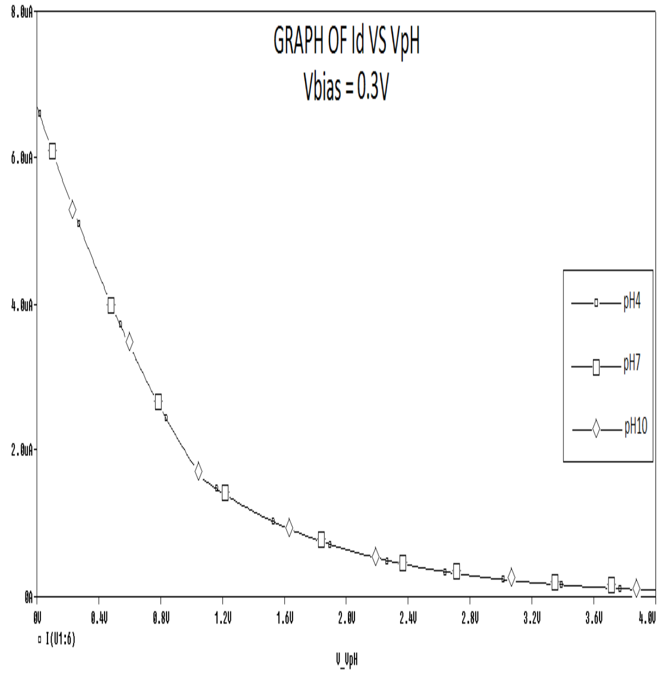

Fig. 7a: Variation of Id with VpH at Vbias of 0.3V

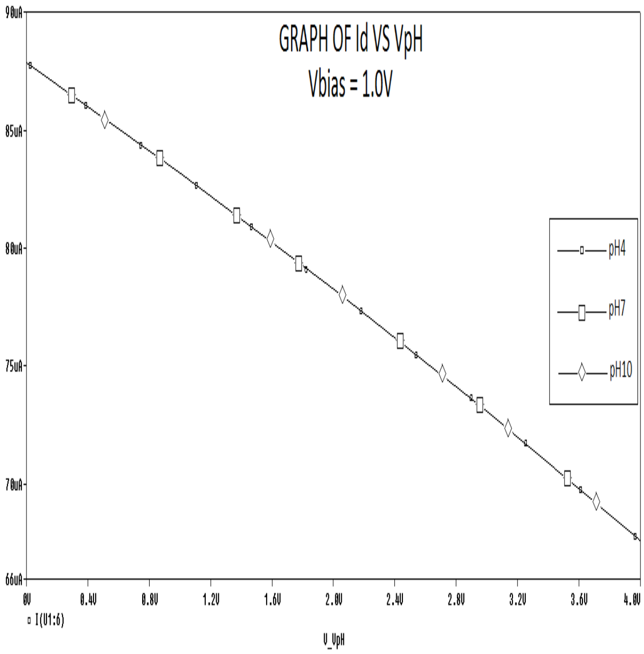

Fig. 7b: Variation of Id with VpH at Vbias of 1.0V

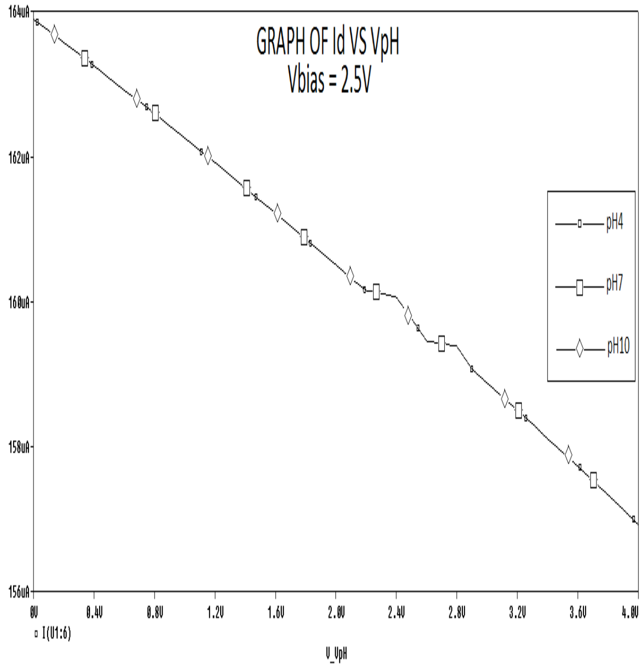

Fig. 7d: Variation of Id with VpH at Vbias of 2.5V

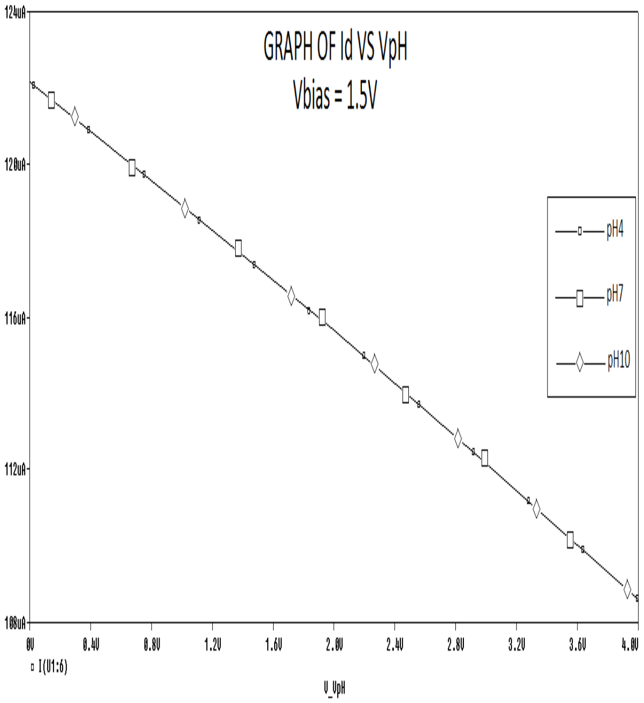

Fig. 7c: Variation of Id with VpH at Vbias of 1.5V

Next, linearity is considered in selecting Vbias. Fig. 8a and Fig. 8b shows plotting of input voltage from signal generator against current flowing through the drain-source junction (Vd) of the ISFET, for different values of pH. By fixing Vbias, the pH value can be measured from 1 to 14. With reference to gap between values of pH, it is found that Vbias of 1.5volt yield better operational linearity than Vbias of 1.0volt. Moreover, it is observed that, irrespective of the pH value, the H+ ISFET saturates at high Vd. At saturation, increasing the input voltage no longer increases the output current. At Vbias of 1.0volt (see Fig. 8a), at pH 14, it can be observed that the output current is already saturated from the beginning, even though the input current is increased. In addition, it can be found that the range of output current for Vbias of 1.0volt (0-28μA) is small relative to that of Vbias of 1.5V (0-70 μA), over the operating range of pH [1-14]. Based on these considerations, Vbias of 1.5volt is selected in preference to Vbias of 1.0 volt, since it linearity performance is better although sensitivity of the latter is slightly better than the former.

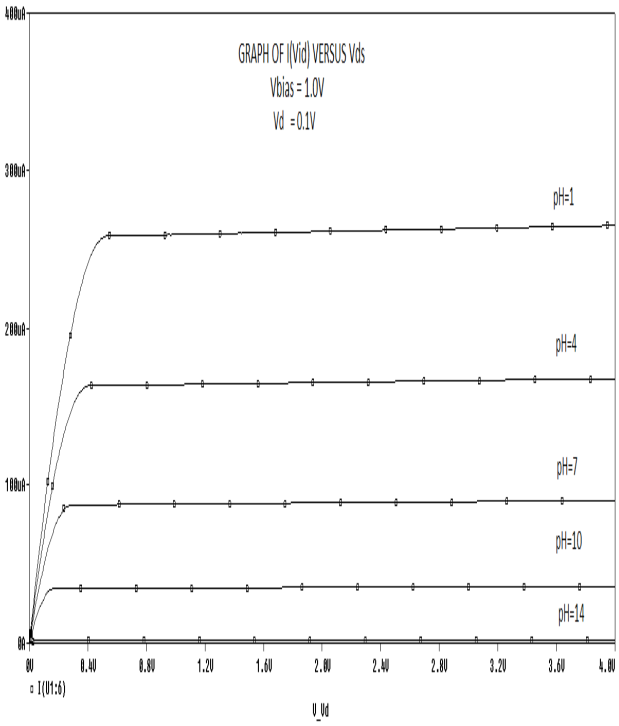

Fig. 8a: Variation of Id with Vd at Vbias of 1.0V

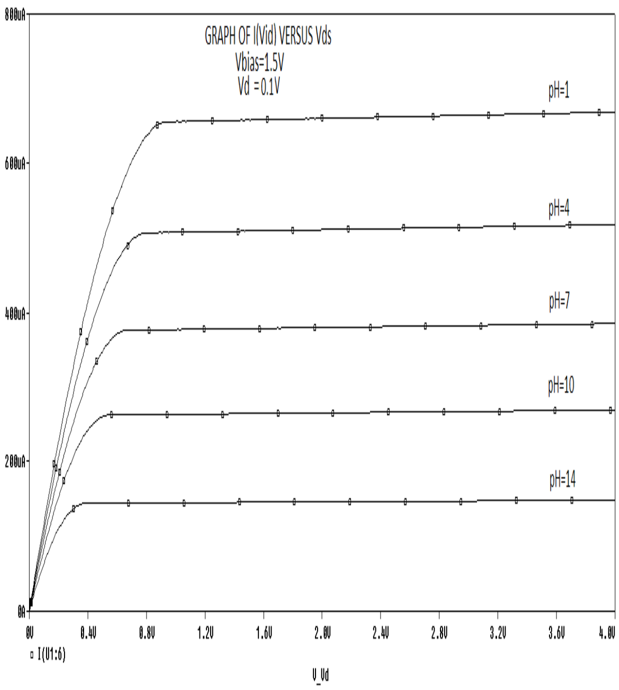

Fig. 8b: Variation of Id with Vd at Vbias of 1.5V

4 CONCLUSION

A new macro model for H+ ISFET is first developed and captured as a sub-circuit block library in PSpice. Before simulation, characteristic of its drain current is matched against that from its mathematical model from previous work, reporting a discrepancy in sensitivity of ±8% for pH [4 7 10]. In addition, our work contributes to the determination of design parameters for an electrolyte insulator interface based Si_3N_4 field effect transistor sensitive to H+ ion, based on macro modeling with PSpice. The optimal drain voltage and Vbias are found to be 0.1volt and 1.5volt respectively. These values are selected with the criteria that the operation characteristic of H+ ISFET to be as linear and sensitive as possible. In selecting drain voltage, it is found that smaller voltage improves the response time and sensitivity of H+ ISFET to chemical input signal, by increasing the reading of drain current and lowering the cut-off voltage. This in turn yields higher sensitivity. A sensitivity of 54.79mV/pH at drain voltage of 0.1volt is reported. In selecting Vbias, both 1.0volt and 1.5volt are found to produce high sensitivity in µA/Vph. However, Vbias of 1.5volt is preferred to 1.0volt for linear change in drain current to pH value.

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