

# Simulating the Drain Current Characteristics of CNTFETs in a Wide Range of the Diameter Values and Polarization Conditions

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## Abstract

In this paper it is simulated the drain current characteristic of the Carbon Nanotube Field Effect Transistor (CNTFET) operating in a wide range of polarization conditions and for different values of the diameter of the Carbon NanoTube (CNT), using a fully empirical current-voltage (I-V) model developed by the author. The empirical approach to modeling is actually a very interesting field of investigation and research for the CNTFETs because it overcomes the drawbacks of the accurate but very complex physical models. The model used in this study is very compact, fast and accurate, without any physical approximation, and then it is particularly suitable for the design of CNTFETs-based electronic circuits. It is validated through comparisons of the I-V calculations with those performed by a very accurate numerical simulator. The model results very useful, fast and accurate to simulate the behavior of the CNTFETs in a wide range of operating conditions and for different values of the diameter.

**Index Terms**— Carbon Nanotubes, Electronic circuits design, Field Effect Transistors, modeling, FETtoy

## I. INTRODUCTION

The most recent developments in electronic devices and circuits technology look forward two main directions. The first one is the direction of the scaling of the well-known silicon (Si) technology until the Moore's law is sustained, to overcome the challenges arising from the so-called second order effects and quantum effects, so difficult to control in nanometer-scale Metal Oxide Field Effect Transistors (MOSFETs) [1]. Anyway, though the scaling trend continues bulk MOSFET will

soon reach its limiting size. Therefore, the second direction the advanced research in electron devices is looking for, deals with the investigation of more futuristic and revolutionary devices as carbon nanotubes field effect transistors (CNTFET) [2].

For this reason, the semiconductor industry together with the academic research is looking for different materials and devices to integrate and perhaps to replace, in the not so far future, the current silicon based technology. To this aim, the carbon nanotube (CNT) based technology, and particularly the CNTFETs, appear to be the most promising alternative due to their exceptional electronic properties [3].

In fact, CNTs are two dimensional graphene sheet rolled into cylindrical shape with diameter in nanometer scale. Depending on the number of sheets rolled, CNT can be either single wall (SW) or multi-walled (MW) and the orientation in which the sheets are rolled, named chirality, allows them both metallic and semiconducting-like behavior.

Metal-like CNTs are able to carry high current density, of the order of  $10 \mu\text{A}/\text{nm}^2$  while standard metal wires have a current carrying capability 1000 times lower.

Moreover, semiconducting-like CNTs, used to fabricate the CNTFET, show an electron mean free path that can exceed  $1 \mu\text{m}$  and then CNTFETs exhibit near-ballistic transport characteristics; furthermore, the mean free path for acoustics phonon scattering has been estimated to be  $300 \text{ nm}$  and for optical phonon scattering is  $15 \text{ nm}$  [4]. These features result in scattering-free, high speed devices and in considerable advantages also over the nanometer-scale MOSFETs devices best performances.

For these very impressive performances, CNTFETs are object of more and more studies nowadays.

However, one of the most important challenges is to model these devices, in particular the current-voltage (I-V) characteristics.

The most used approach to I-V modeling is based on the solution of the set of equations describing the generation, the transport and the control by applied voltages of the charge carriers inside the device, i.e. based on the dispersion relation of the graphene, the non-equilibrium Green's function and the Schroedinger and Poisson equations (SP solvers) [5].

The solution of this set of physical equations is generally performed numerically to obtain accurate results but such models are so complex and oriented to the analysis of devices; they are not useful for circuits design due to their complexity. In order to obtain quite simple and compact models a number of approximations are needed resulting in lower accuracy of the models [6] especially for high drain-source voltages, i.e.  $V_{\text{DS}} > 1\text{V}$ , and for different values of the diameter of the CNT.

Due to these considerations, the author has developed a new, very fast, simple and accurate model of CNTFETs [7]. The model is based on an empirical approach in past successfully applied by the author to the characterization of Gallium Arsenide (GaAs) Metal Semiconductor Field Effect Transistors (MESFET) [8, 9]. The model is applied for the first time in this paper to model also the I-V characteristics of the CNTFETs having a diameter ranging from  $1 \text{ nm}$  to  $5 \text{ nm}$  and operating in a wide range of polarization conditions.

No S-parameters and no parasitic resistances measurement is required by the model.

Moreover, the model is suitable to fit I-V curves of the device either measured or calculated by other more complex models, with the aim to replace them for circuits design purposes, without losing accuracy.

In fact, any software for circuits design needs analytical models of the devices (transistors) used to build circuits [10]. Simpler and more accurate are the models of the devices, faster and more accurate is the design of electronic circuits.

The paper is organized as follows: in section II the new empirical model developed by the author is deeply described; in section III a simulation session is conducted and the model is verified through the comparison of the modeled I-V characteristics of single-wall (SW) MOSFET-like CNTFETs with the same curves obtained by using the accurate numerical simulator FETtoy [11]. To this aim, four CNTFETs have been simulated, with different values of the diameter and operating in a wide range of drain-source voltage. Conclusions are in section IV.

## II. MODEL DESCRIPTION

### A. *The empirical approach to modeling*

An empirical I-V model is developed by using mathematical functions whose graphical representation is similar to the measured I-V curves [7-9]. The use of empirical parameters inside mathematical equations enables the modelled curves to be matched to the measured curves as well as possible. To determine the value of these empirical parameters the absolute error between measured and calculated drain current values is minimized and the parameter extraction procedure is so performed.

In terms of computability, an empirical model is much more easily tailored to fast convergence performance, computing time and accuracy and doesn't require any approximation. On the other hand, this kind of model is at a first glance far from the intuition of the physical mechanisms governing the behavior of the device. Consequently, a significant attention is required to determine the values of the empirical parameters, especially of their initial estimation to start the extraction procedure by searching for the best fit between measured and modelled current values, as above mentioned.

Moreover, in other I-V models of CNTFETs so as of all electronic devices, the current is calculated as a function of internal voltages, i.e. considering the voltage drop due to the source and drain parasitic resistances. This is a significant limitation because of these resistances depend on the bias condition and approximate estimation of their value is generally used. On the other hand, the accurate measurement and modeling of such resistances is so difficult and so time-consuming making the models necessarily approximated and/or not very useful.

This problem is overcome in the proposed model by using the external voltages to fit the I-V measured curves.

Finally, the current of the CNTFETs is strongly dependent on the chirality, diameter, channel length, threshold voltage, leakage currents and on the bias (operating) conditions of the device and generally models accurate for any of these

situations are not yet been proposed.

The new proposed empirical model is accurate for any of these parameters/conditions and as for low as for high power CNTFETs, as shown in the simulation results (Section III).

### B. New model features and description

The proposed new drain current model equation for the CNTFET is:

$$I_{DS} = [I_{DSS0} + G_1 V_G + K_2 V_G^2](\lambda_0 + \lambda_1 V_{DS})[\tanh(\alpha V_{DS})]^M \quad (1)$$

$V_{GS}$  is the gate-source voltage,  $V_{DS}$  is the drain-source voltage and  $V_t$  is the threshold voltage of the device. Moreover:

$$V_G = V_{GS} - V_t \quad (2)$$

$$V_t = V_{th} + \gamma V_{DS} V_{GS} \quad (3)$$

$$\alpha = a_0 + a_1 V_{GS} + a_2 V_{GS}^2 + a_3 V_{GS}^3 \quad (4)$$

The empirical parameters  $I_{DSS0}$ ,  $G_1$ ,  $K_2$ ,  $V_{th}$ ,  $\lambda_0$ ,  $\lambda_1$ ,  $\gamma$ ,  $M$ ,  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$  have to be extracted by dividing them into two batches, making more fast and accurate the extraction procedure based on the search of the best fit (i.e. the minimum error) between the measured and the modeled current values.

Firstly,  $I_{DSS0}$ ,  $G_1$ ,  $K_2$ ,  $V_{th}$ ,  $\lambda_0$ ,  $\lambda_1$ ,  $\gamma$ , are determined; then  $M$ ,  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$  are determined, as explained subsequently.

Moreover, the extraction is easily performed because of the calculation of the initial values of the empirical parameters by considerations relevant to the physical/electrical behavior of the device to be characterized.

The hyperbolic tangent function has the shape of the typical I-V characteristics and then it is a very useful function to the aim of empirical modeling of the linear and knee region [7-9]. The parameters  $\alpha$  and  $M$  allow the best fit between the hyperbolic tangent function and measured current values in the knee region and in the linear region, here modifying the behavior of the hyperbolic tangent function.

The term  $(\lambda_0 + \lambda_1 V_{DS})$  models the drain control over the CNTFET current in the saturation region while the term

$(I_{DSS0} + G_1 V_G + K_2 V_G^2)$  models the gate control over the CNTFET current. In fact, it is a more general expression of the approximated FET equation:  $I_{DS} = I_{DSS}(1 - V_{GS}/V_t)^2$

Equation (3) models the shift of the threshold voltage at zero bias,  $V_{th}$ , due to a number of conduction phenomena so difficult to accurately model with physical equations.

This interpretation of the terms in equation (1) allows a quite simple initial estimation of the values of the empirical parameters to be extracted allowing a fast and accurate convergence for the calculation of their final values.

In fact, as above mentioned, the extraction procedure to calculate the values of the empirical parameters searches for the best fit (i.e. the minimum error) between the reference and the modeled  $I_{DS}$ - $V_{DS}$  curves. Therefore, an initial estimation of the empirical parameters of the model is needed in order to start the extraction routine, and the initial estimation is facilitated by the meaning of the terms of the model that we have just explained.

Therefore,  $I_{DSS0}$ ,  $K_2$  and  $G_I$  are estimated as the coefficients of the second-order polynomial interpolating the maximum saturation drain-source reference current ( $I_{DSS}$ ) as a function of the voltage  $V_{GS}$ .

Initial values of  $\lambda_0$ ,  $\lambda_I$ , and  $\gamma$ , should be set equal to zero due to the electrical behavior of an ideal CNTFET. In fact, in an ideal CNTFET, there is no shift in the threshold voltage ( $\gamma=0$ ) and there is a full gate control over the current (i.e. there is no drain control over the current in the saturation region resulting  $\lambda_0 = \lambda_I = 0$ ).

The initial value of M parameter can be easily estimated considering that it is a fine-tuning parameter that modifies the hyperbolic tangent shape especially in the knee region of I-V curves. Therefore, giving M = 1 as initial value of M to start the parameter extraction routine, is a useful choice.

The initial values of coefficients  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$  of the parameter  $\alpha$  can be calculated following two approaches based on two physical approximations.

Both approaches derive from the observation that the hyperbolic tangent function approaches to unity when its argument is large enough, i.e.  $\alpha V_{DS} \geq 6$ . Moreover, the approximated behavior of the current of the CNTFET in the saturation region (i.e. for  $V_{DS} \geq V_{DSAT}$  being  $V_{DSAT}$  the saturation drain-source voltage) is almost constant. Therefore, it is correct to assume that  $\tanh(\alpha V_{DSAT}) \rightarrow 1$  and, then,  $\alpha V_{DSAT} \geq 6$ .

According to these considerations, it is possible to follow two ways to estimate the coefficients  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$ .

The first, rough, but useful approximation consists to neglect the dependence of  $V_{DSAT}$  on  $V_{GS}$ . In such a way, it is possible to estimate  $V_{DSAT}$  by the  $I_{DS}-V_{DS}$  curve for  $V_{GS} = 0$  as the value of  $V_{DS}$  corresponding to the end of the knee region, and subsequently to estimate  $a_0 = 6/V_{DSAT}$ ,  $a_1 = a_2 = a_3 = 0$ .

The second way to determine the initial values of the coefficients  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$  is more accurate but also more time consuming. It can be performed determining approximately the  $V_{DSAT}$  corresponding to many values of  $V_{GS}$  and by interpolating with a third-order polynomial the values  $6/V_{DSAT}$ . The coefficient of the interpolation polynomial is the initial estimation of the required  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$  parameters, to start the minimization routine.

Finally, the initial value of the threshold voltage is assumed as a half of the band gap  $E_{bg}$  of the CNT acting as a channel of the CNTFET as [10]:

$$V_{th} \simeq \frac{E_{bg}}{2e} = \frac{aV_{\pi}}{ed} \simeq \frac{0.436}{d(nm)} \quad (5)$$

being:  $e$  the electron charge,  $a \approx 0.144$  nm the length of the carbon-carbon bond,  $V_{\pi} \approx 3.033$ eV is the energy of the  $\pi-\pi$  bond and  $d$  the diameter of the CNT.

The extraction routine which starts with these initial values of the empirical parameters results fairly quick, running in a few seconds, and unique.

### III. RESULTS

The previously described empirical model has been validated by comparisons with reference I-V curves obtained by the numerical model implemented in the FETtoytool [11]. Moreover, it has been used to simulate the I-V characteristics of devices having

different diameter values,  $d$ . Different values of the CNT diameter,  $d$ , have significance effects on  $I_{DS}$  due to the energy gap of all sub bands are inversely proportional to the CNT diameter [1].

The calculations have been performed for MOSFET-like CNTFETs having oxide thickness  $t=1.5nm$  and SiO<sub>2</sub> as gate dielectric (dielectric constant  $k = 3.99$ ).

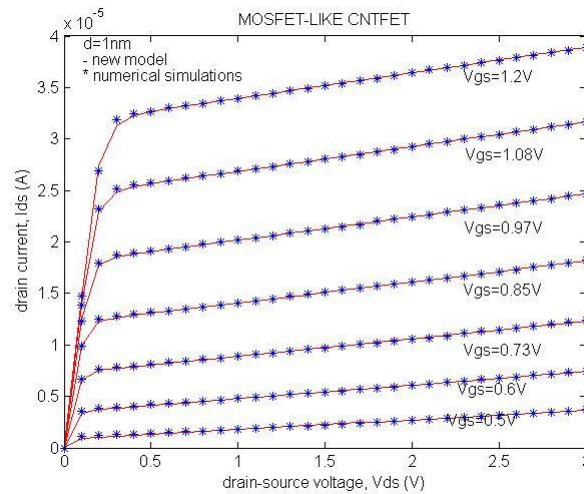
Fig. 1 shows the  $I_{DS}$ - $V_{DS}$  curves for different values of  $V_{GS}$  and for  $V_{DS}$  up to 3V for a CNTFET having a diameter  $d=1nm$ .

In fig. 2 the drain current versus the gate voltage ( $I_{DS}$ - $V_{GS}$ ) curves are plotted for different values of  $V_{DS}$ .

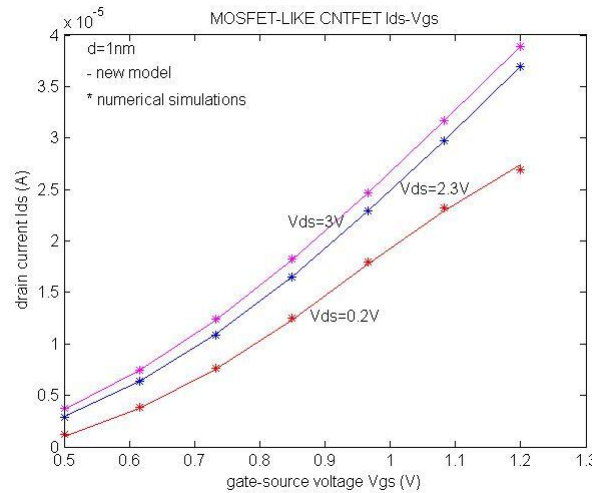
The mean percentage error between the  $I_{DS}$  calculations performed by the FETtoy simulator and by the new model is about of 0.7%.

In table I there are the values of the empirical parameters calculated by the minimization routine. These values hold for fig. 1 and 2.

It is evident that the new model  $I_{DS}$  calculations for low and high voltages applied are closed to those by FETtoy simulator.



**Fig. 1.  $I_{DS}$ - $V_{DS}$  curves for  $d = 1nm$  with different values of  $V_{GS}$**



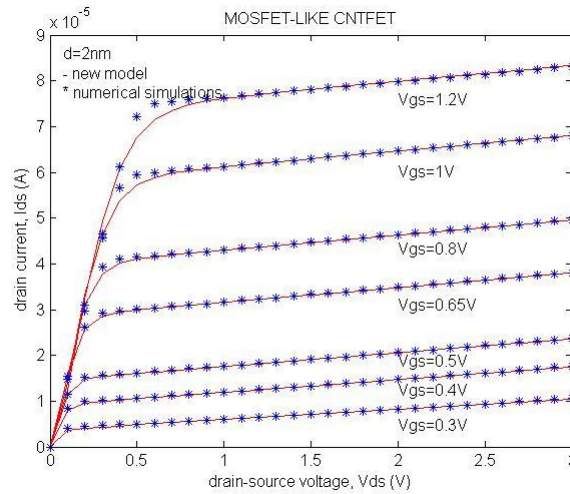
**Fig. 2.  $I_{DS}$ - $V_{GS}$  curves for  $d = 1nm$  with different values of  $V_{DS}$**

Fig. 3 shows the  $I_{DS}$ - $V_{DS}$  curves for different values of  $V_{GS}$  and for  $V_{DS}$  up to 3V for a CNTFET having diameter  $d=2nm$ .

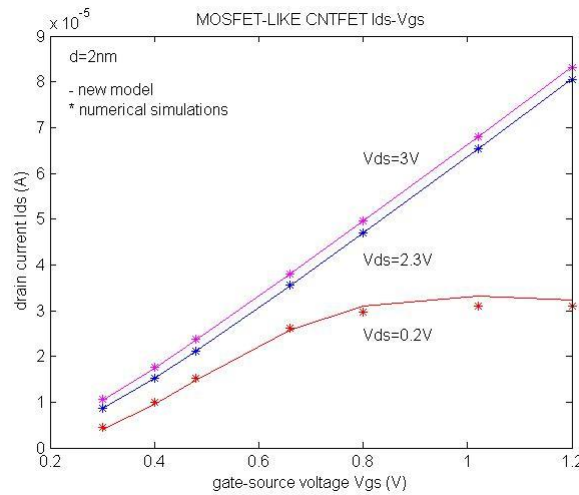
In fig. 4 the drain current versus the gate voltage ( $I_{DS}$ - $V_{GS}$ ) curves are plotted for different values of  $V_{DS}$ .

The mean percentage error between the  $I_{DS}$  calculations performed by the FETtoy simulator and by the new model is about of 0.9%.

In table II there are the values of the empirical parameters calculated by the minimization routine. These values hold for fig. 3 and 4.



**Fig. 3.  $I_{DS}$ - $V_{DS}$  curves for  $d = 2 \text{ nm}$**



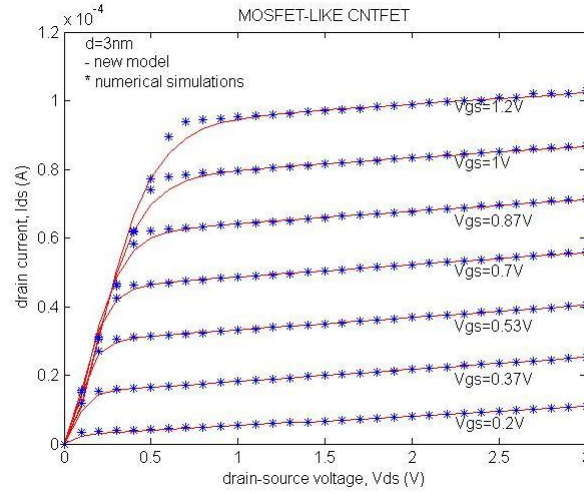
**Fig. 4.  $I_{DS}$ - $V_{GS}$  curves for  $d = 2 \text{ nm}$**

Fig. 5 shows the  $I_{DS}$ - $V_{DS}$  curves for different values of  $V_{GS}$  and for  $V_{DS}$  up to 3V for a CNTFET having diameter  $d = 3nm$ .

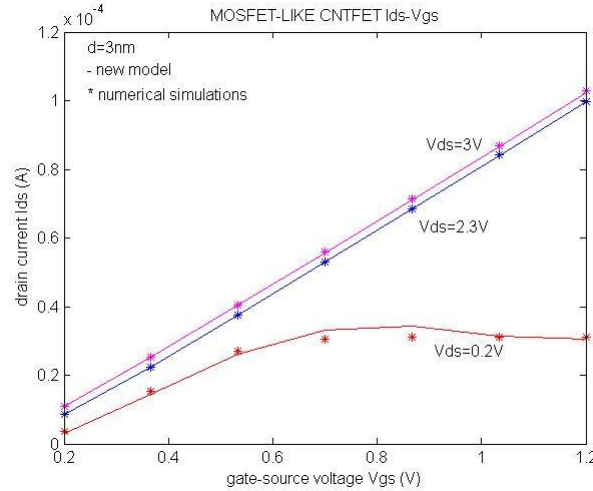
In fig. 6 the drain current versus the gate voltage ( $I_{DS}$ - $V_{GS}$ ) curves are plotted for different values of  $V_{DS}$ .

The mean percentage error between the  $I_{DS}$  calculations performed by the FETtoy simulator and by the new model is about of 1.61%.

In table III there are the values of the empirical parameters calculated by the minimization routine. These values hold for fig. 5 and 6.



**Fig. 5.  $I_{DS}$ - $V_{DS}$  curves for  $d = 3$  nm**



**Fig. 6.  $I_{DS}$ - $V_{GS}$  curves for  $d = 3$  nm**

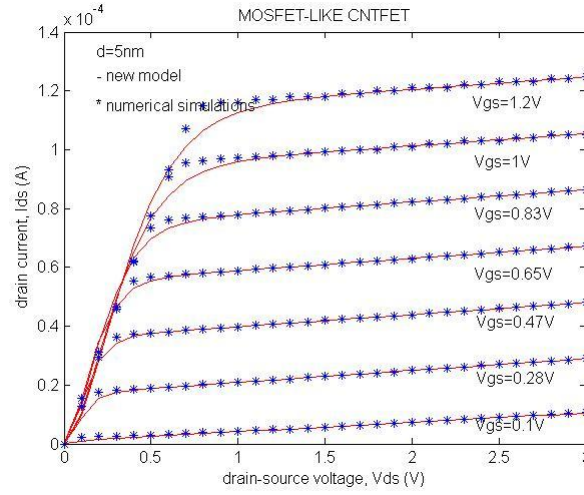
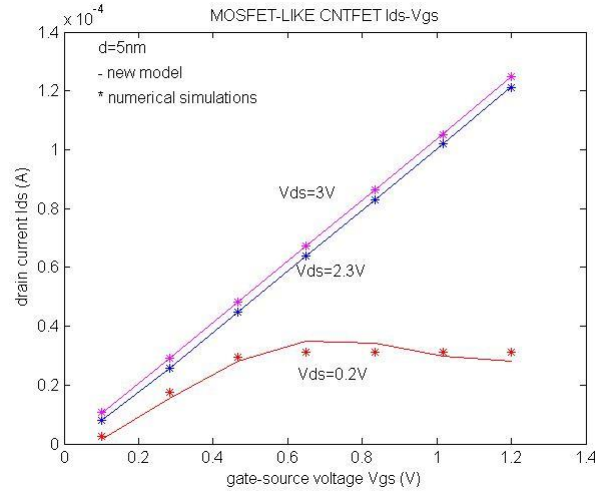
Fig. 7 shows the  $I_{DS}$ - $V_{DS}$  curves for different values of  $V_{GS}$  and for  $V_{DS}$  up to 3V for a CNTFET having diameter  $d = 5$  nm.

In fig. 8 the drain current versus the gate voltage ( $I_{DS}$ - $V_{GS}$ ) curves are plotted for different values of  $V_{DS}$ .

The mean percentage error between the  $I_{DS}$  calculations performed by the FETtoy simulator and by the new model is about of 2.6%.

In table IV there are the values of the empirical parameters calculated by the minimization routine. These values hold for fig. 7 and 8.




**Fig. 7.  $I_{DS}$ - $V_{DS}$  curves for  $d = 5$  nm**

**Fig. 8.  $I_{DS}$ - $V_{GS}$  curves for  $d = 5$  nm**
**Table I – Empirical parameters values for different values of the polarization gate-source voltage  $V_{GS}d = 1$  nm**

$V_{GS}$ (V)	$I_{DSS0}$ ( $\mu A$ )	$G_1$ ( $e^{-2}S$ )	$K_2$ ( $\mu A/V^2$ )	$\lambda_0$ ( $e^{-6}$ )	$\lambda_1$ ( $e^{-6} V^{-1}$ )	$\alpha$ ( $V^{-1}$ )	M	$V_{th}$ (V)	$\gamma$ ( $V^{-1}$ )
0.5	$1.59e^3$	0.86	-14.77	0.87	0.93	24.33	1.95	0.44	-0.07
0.6	$1.59e^3$	0.86	-14.77	3.46	1.32	20.90	1.95	0.44	-0.07
0.73	$1.59e^3$	0.86	-14.77	7.20	1.70	17.58	1.95	0.44	-0.07
0.85	$1.59e^3$	0.86	-14.77	12.06	2.03	14.50	1.95	0.44	-0.07
0.97	$1.59e^3$	0.86	-14.77	17.94	2.24	11.80	1.95	0.44	-0.07
1.08	$1.59e^3$	0.86	-14.77	24.48	2.39	9.62	1.95	0.44	-0.07
1.2	$1.59e^3$	0.86	-14.77	31.47	2.47	8.10	1.95	0.44	-0.07

**Table II – Empirical parameters values for different values of the polarization gate-source voltage  $V_{GSd} = 2 \text{ nm}$** 

$V_{GS} (V)$	$I_{DSS0} (\mu A)$	$G_1 (e^{-2} S)$	$K_2 (\mu A/V^2)$	$\lambda_0 (e^{-6})$	$\lambda_1 (e^{-6} V^{-1})$	$\alpha (V^{-1})$	M	$V_{th} (V)$	$\gamma (V^{-1})$
0.3	$1.9e^3$	1.65	-63	3.72	2.26	18.59	1.62	0.24	-0.3
0.4	$1.9e^3$	1.65	-63	9.18	2.78	14.86	1.62	0.24	-0.3
0.5	$1.9e^3$	1.65	-63	14.60	3.02	12.40	1.62	0.24	-0.3
0.65	$1.9e^3$	1.65	-63	28.44	3.22	8.32	1.62	0.24	-0.3
0.8	$1.9e^3$	1.65	-63	39.80	3.27	6.27	1.62	0.24	-0.3
1	$1.9e^3$	1.65	-63	57.99	3.32	4.38	1.62	0.24	-0.3
1.2	$1.9e^3$	1.65	-63	73.07	3.35	3.48	1.62	0.24	-0.3

**Table III – Empirical parameters values for different values of the polarization gate-source voltage  $V_{GSd} = 3 \text{ nm}$** 

$V_{GS} (V)$	$I_{DSS0} (\mu A)$	$G_1 (e^{-2} S)$	$K_2 (\mu A/V^2)$	$\lambda_0 (e^{-6})$	$\lambda_1 (e^{-6} V^{-1})$	$\alpha (V^{-1})$	M	$V_{th} (V)$	$\gamma (V^{-1})$
0.2	$0.9e^2$	2.05	-83	2.50	2.78	12.20	1.67	0.15	0.45
0.37	$0.9e^2$	2.05	-83	14.6	3.52	9.82	1.67	0.15	0.45
0.53	$0.9e^2$	2.05	-83	29.54	3.65	7.70	1.67	0.15	0.45
0.7	$0.9e^2$	2.05	-83	44.80	3.68	5.84	1.67	0.15	0.45
0.87	$0.9e^2$	2.05	-83	6.03	3.71	4.37	1.67	0.15	0.45
1.03	$0.9e^2$	2.05	-83	7.58	3.72	3.35	1.67	0.15	0.45
1.2	$0.9e^2$	2.05	-83	9.14	3.76	2.85	1.67	0.15	0.45

**Table IV – Empirical parameters values for different values of the polarization gate-source voltage  $V_{GSd} = 5 \text{ nm}$** 

$V_{GS} (V)$	$I_{DSS0} (\mu A)$	$G_1 (e^{-2} S)$	$K_2 (\mu A/V^2)$	$\lambda_0 (e^{-6})$	$\lambda_1 (e^{-6} V^{-1})$	$\alpha (V^{-1})$	M	$V_{th} (V)$	$\gamma (V^{-1})$
0.1	$100e^3$	6.75	-114	0.91	3.20	9.45	1.65	0.09	0.016
0.28	$100e^3$	6.75	-114	16.8	4.06	7.93	1.65	0.09	0.016
0.47	$100e^3$	6.75	-114	35.6	4.13	6.38	1.65	0.09	0.016
0.65	$100e^3$	6.75	-114	54.7	4.15	4.90	1.65	0.09	0.016
0.83	$100e^3$	6.75	-114	73.8	4.16	3.65	1.65	0.09	0.016
1	$100e^3$	6.75	-114	93.1	4.11	2.74	1.65	0.09	0.016
1.2	$100e^3$	6.75	-114	112.2	4.18	2.31	1.65	0.09	0.016

The total mean percentage error between current calculations performed by the FETtoy simulator and by the new model is less than 1.5%

#### IV. CONCLUSIONS

In this paper a new, very fast and accurate empirical model of CNTFETs has been described and applied to simulate the I-V characteristics of CNTFETs having

different values of the diameter and operating in a wide range of polarization conditions.

The model and simulation results have been validated by comparisons with calculations obtained by the numerical simulator FETtoy.

CNTFETs having a diameter ranging from 1nm to 5nm, i.e. having very different current values, have been successfully simulated, in a wide range of operating conditions.

The percentage mean error is less than 1.5% for all I-V calculations performed for different values of  $V_{GS}$  and of the CNT diameter, as for low as for high bias voltages.

The need for a procedure of extraction of the model empirical parameters appears as the only drawback of the model. Anyway, this paper demonstrates that it is easily possible to perform an estimation of the initial values of the model parameters to start the extraction routine very close to their final values, by physical considerations. In this way, the extraction routine runs easily, quickly and accurately calculates the empirical parameters of the model.

Finally, no S parameters and no parasitic resistances have to be determined.

We can conclude that the fully empirical approach is very suitable for the design of analog and digital circuits based on CNTFETs. Moreover, the new empirical model due to its accuracy and compactness can replace the more complex and time consuming SP-solver in the design of complex circuits using CNTFETs with any dimension of the diameter and operating in a wide range of polarization conditions.

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