Verilog-A Behavioral Model of Hydrogen Bonding Network

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Abstract - **Information processing requires new approaches and circuits. Novel algorithms and devices are needed to emulate the operation of bioobjects such as DNA, neuron networks, and proteins with their hydrogen bonding networks. In the present paper a circuit to imitate the proton transfer in hydrogen bonding network is developed. It is modeled in Cadence CAD system using Verilog-A language which is compared to already investigated Matlab model. Based on the behavioral model a DC and transient analyses are performed. The results show the modeled circuit is similar to a current mirror or an amplifier.**

Keywords – **Hydrogen bonding network, microelectronic circuits, proton transfer, Verilog A, Behavioral modeling.**

I. INTRODUCTION

Processing of information would become a real challenge in the near future in the context of the constantly increasing acquisition of information. The complexity of the problems related to information processing needs novel concepts opening the horizon of new non-standard ideas. The methods and algorithms that originate from the nature prove to be a promising approach.

The architecture of the human brain and the natural neuron networks [1] serve as a source of ideas and approaches for evolving conventional microelectronics. On its basis are developed series of artificial neuron networks to solve complex computational problems. Their genetic algorithm is suitable to represent various nonlinear functions applicable to micro- and nanoelectronics.

In addition, the proteins and their hydrogen bonding networks can also have functions applicable to microelectronics. For example, the protein Bacteriorhodopsin (bR) [2] is suitable for microelectronics purposes as it transports protons via its own hydrogen bonding networks. The signal transfer (proton transfer) is investigated also for other hydrogen bonding networks (HBN), e.g. the HBN extracted from β-lactamase protein [3]. Its proton transport is described by Marcus theory [4] and protein electrostatic theory. It has been proved that the proton transfer parameter (the proton current, respectively) and the donor/acceptor electrostatic potentials depend on the pH that changes with the electrostatic potential of the donors and acceptors. Based on its hydrogen bonding network a block-element circuit [5] that models its behavior is realized in Matlab [6]. In the model circuit each donor and acceptor is substituted by electronic block-element; the proton transfer parameter is juxtaposed to electrical current and the electrostatic potential of donor/acceptor atom is juxtaposed to electrical voltage. The preformed static and dynamic simulations showed that the circuit works similarly to current mirror, amplifier or decoder, i.e. similarly to real electronic device. Logical next step is to make a model of the hydrogen bonding network using CADENCE CAD system using Verilog A hardware description language.

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II. CIRCUITS

The hydrogen bonding network in Figure 1 [5] shows the connections between each heavy atom.

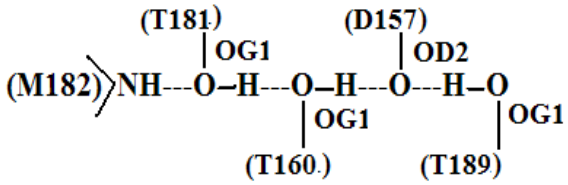


FIGURE. 1 HYDROGEN BONDING NETWORK (M1) WITHOUT INVOLVING OF WATER MOLECULES. (M182) IS METHIONINE RESIDUE, OG1 IS HYDROXYL OXYGEN OF THREONINE RESIDUES (T160,181,189), OD2 IS CARBOXYL OXYGEN OF ASPARTIC ACID RESIDUE (D157)

Here the M182N and K192NZ residuums have strong donor properties and hence can be analogous to microelectronics current sources. The D157 residuum is a strong acceptor and it can be analogous to a microelectronics adder of two signals; it also serves as a circuit output. The other circuit elements are modeled as thee- and four-terminal block-elements. Each of them has equal input and output voltages and different currents.

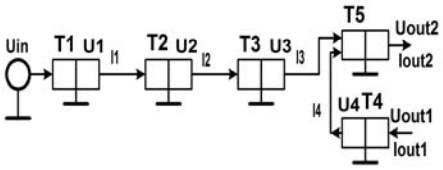


FIGURE 2. ELECTRIC CIRCUIT FUNCTIONALLY ANALOGOUS TO HBN M1.

On the figure 2 is illustrated the circuit analogous to the hydrogen bonding network that is realized as combination of thee- and four-terminal block-elements which is investigated in [5]. The I–V characteristics of the block-elements are analogous to K–V characteristics of the hydrogen bonds in [5]. The current (I) of each block-element represents the proton transfer parameter (K) of each hydrogen bond and the voltage of each block-element represents the donor (acceptor) electrostatic potential (El. pot. [V]).

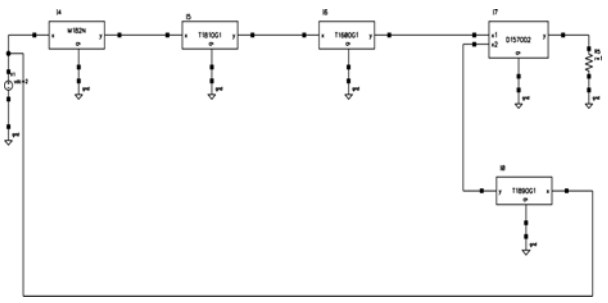


FIGURE 3. CIRCUIT OF HBN M1 IN CADENCE.

The circuit of Figure 3 is developed in Cadence [7]. It is similar to the circuit from Figure 2. The block-elements are described in Verilog A hardware description language [8]. The current and voltage relations are expressed by polynomials of different orders. Some of the block-element equations in Verilog A are given below. The rest of the equations are similar to these.

Equations of block-element T1 analogous to M182N:

$U_{in} = U_1$
$U_1 = [-2.1:0.1:2.65];$

The range of the input voltage is defined by the potential on M182N.

$I_1 = 8*10^{-5}*U_1^4 - 7*10^{-5}*U_1^3 - 0.001*U_1^2 + 0.0048*U_1 + 0.2516;$

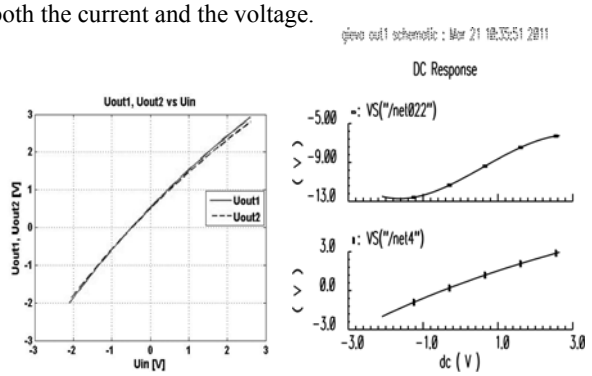
Verilog A code:

```
// VerilogA for Verilog, M182N, veriloga

`include "constants.h"
`include "discipline.h"

module M182N (x, y, g);
inout x, y, g;
electrical x, y, g;
electrical Vin;
 analog
  begin

  V(Vin) <+ V(x, g);
  V(y) <+ V(Vin);
  I(x, y) <+ 8*10e-5*V(y)*V(y)*V(y)*V(y)-7*10e-5*V(y)*V(y)*V(y)-
0.001*V(y)*V(y)+0.0048*V(y)+0.2516;

  end
        endmodule
```

III. DC ANALYSES

The DC analysis is performed using input voltage from -2 to +3 V in Cadence.

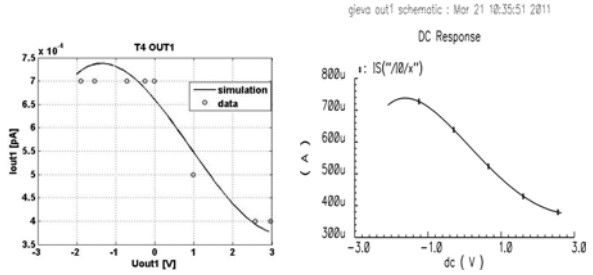
The simulations show that the results from Cadence simulations are similar to the results from Matlab simulations. The output voltages are linear with respect to input voltage. The difference between Cadence and Matlab simulations is in the amplitude and the form of the voltage in the second output (Figure. 4b). It arises from the Cadence limitations. The nature of the Cadence circuit simulator does not allow for simultaneous description of both the current and the voltage.



a) b)

FIGURE 4. OUTPUT VOLTAGES AT OUTPUT 1 AND OUTPUT 2 VS. INPUT VOLTAGE.

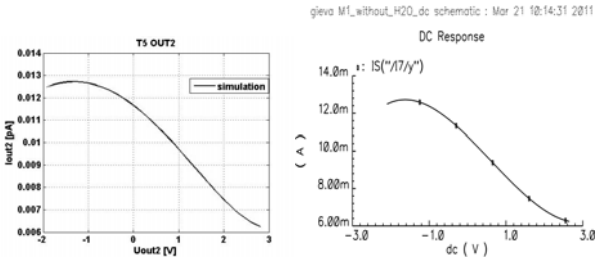
The output currents simulation of the circuit modeled in Cadence are also comparable to the results obtained with Matlab (Figure. 5a, b). From both figures, it can be seen that the form of the curves is similar. The difference between the diagrams is in the value of the current. The dimension of Iout1 current in Matlab model is in [pA] while the current in Cadence model is in [uA] dimension. The difference in the orders of the current is due to Spectre simulator restrictions imposed by the 0.35-um technology design kit that is used in the circuit simulations. However, the form of curves is similar. The circuit simulated in Cadence reproduces the behavior of the Matlab circuit and the functions of the hydrogen bonding network functions.



a) b)

FIGURE 5. I-V CHARACTERISTIC OF BLOCK-ELEMENT T4 (THE FIRST OUTPUT OF THE MICROELECTRONIC CIRCUIT).

The situation is the same with the currents from output 2 modeled with Matlab and Cadence and shown in Figure. 6a, b. The form of the curves is similar and the difference is again in the dimension – [pA] and [mA] respectively for Matlab and Cadence simulations.



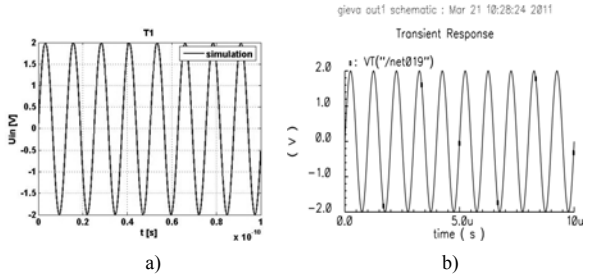
a) b)

FIGURE 6. I-V CHARACTERISTIC OF BLOCK-ELEMENT T5 (THE SECOND OUTPUT OF THE MICROELECTRONIC CIRCUIT).

The I–V characteristics of both outputs (Figure. 5b and 6b) can be separated in two areas. When the voltages are in the interval from -2 to -1 [V] — the output currents do not change significantly. Hence, the circuit can operate as current mirror which generates two different currents in its outputs. When the output voltages are greater than –1 [V] (second operating area) – the circuit has properties similar to an amplifier.

IV. TRANSIENT ANALYSES

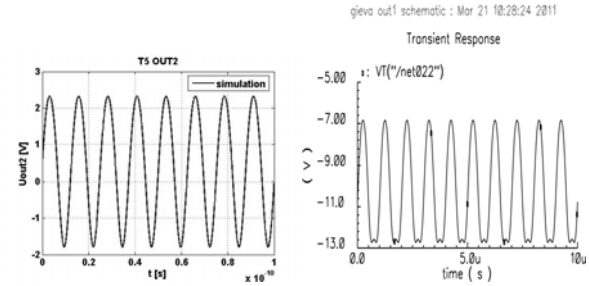
The transient analyses is performed by feeding sine-shaped input voltage with amplitude of +2 [V] and frequency of 1 [MHz]. The results are given in Figures 7b – 10b. The maximum working frequency of the hydrogen bonding network is around 100 GHz like in Matlab simulations but Cadence uses 0.35 um technology that restricts frequency of simulations to 1 [MHz]. That is the basic difference Verilog-A circuit and the hydrogen bonding network simulated in Matlab.



a) b)

FIGURE 7. INPUT VOLTAGE VS. TIME.

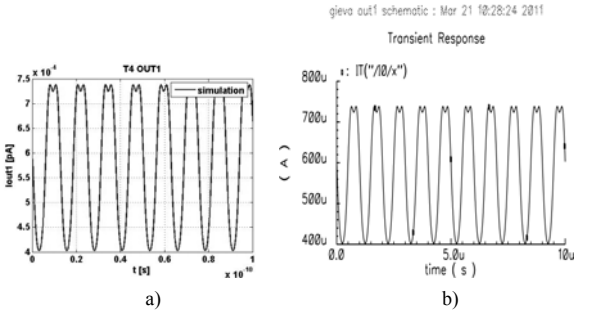
The input voltages in both simulations (Figure. 7a, b) have sinusoidal wave form and equal amplitude, but it has different frequency. The voltage from output 1 is with similar characteristics to the input voltage that is why it is not shown. There is a difference at the second output (Figure. 8a, b). It is due to simulation program specifics.



a) b)

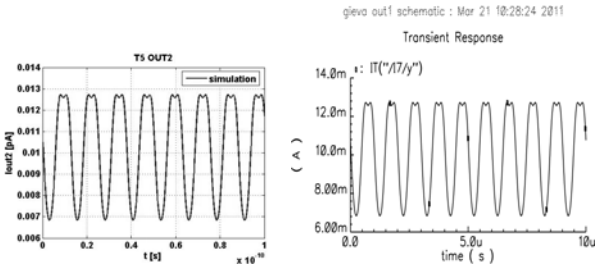
FIGURE 8. OUTPUT VOLTAGE AT SECOND OUTPUT VS. TIME.

From both simulations Iout1 is with similar form (Figure. 9 a, b). The differences are in the frequency and the dimensions. The situation with Iout2 is similar in both simulations (Figure. 10 a, b) the differences are the same; the circuit realized in Cadence behaves like the circuit modeled in Matlab.



a) b)

FIGURE 9. OUTPUT CURRENT AT FIRST OUTPUT VS. TIME.



a) b)

FIGURE 10. OUTPUT CURRENT AT SECOND OUTPUT VS. TIME.

A distinctive feature of the output currents is that they are always positive and they are independent from positive or negative semi-sine of the input voltage. Hence, this circuit can operate as decoder.

V. CONCLUSION

The tested circuit well represents the properties of the hydrogen bonding network. The development behavioral model and the DC and transient analyses showed that the network is analogous to current mirror, amplifier or decoder. Hence, it can be concluded that based on the proteins and their hydrogen bonding networks new devices and algorithms for information processing can developed.

VI. ACKNOWLEDGEMENT

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