Behavioral modeling of circuit functional analogous to hydrogen bonding network with water molecules

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Abstract - **In the present paper is considered a circuit which comprises block-elements, analogous to behavioral of hydrogen bonding network extracted from the protein β-lactamase and containing water molecules. The circuit is described using Verilog-A language. The DC and transient analysis have been made in the environment Cadence and obtained results are compared with previous results from Matlab. It is proved that the circuit could work as a differential amplifier, CMOS power amplifier and others.**

Keywords – **proteins, hydrogen bonding network, Verilog-A, β-lactamase, proton transfer**

I. INTRODUCTION

Following the rapid development of electronics in recent years, it is necessary to look for alternative solutions. More and more are talk about nanotechnology [1] bioelectronics [2] and molecular electronics [3].

Another type of an alternative technology is biomolecular electronics [4]. It aims to use organic compounds as an environment for transmission or processing of electrical signals. One of the main structures that are used are proteins. They are studied different proteins with different structures and properties. Some proteins such as GFP [5] and Cytochrome C [6] observed electrical transfer, while others like Bacteriorhodopsin [7] observed proton transfer. However, in all of them is transmit the signal. This is the main reason why they are tested for application in electronics.

The bacteriorhodopsin is one of the most studied membrane proteins. It is used for different biodevices as optical memory [8], biomolecular electronic devices [9] and others.

A microelectronic circuit is similar to hydrogen bonding network which is extracted from the protein β-lactamase. Each block-element is coded into Cadence [10] and is described by a behavioral description language Verilog-A [11]. Then are made analyses of the results and they are compared with the same previous results in Matlab [12], the results are taken from [13].

The proton transport in the studied network is described by Marcus theory [14]. It has been shown that proton transfer parameter depends on the change in the environment (pH), which changes the electrostatic potential of donors and acceptors. In this circuit, each donor and acceptor is substituted by an electronic block-element, parameters of proton transfer are compared with the electrical current and the potential of the atom is juxtaposed to electrical voltage. The DC and transient simulation of testing circuit show that it behaves like real electronic devices.

After the creation of block-elements, which imitate the functions of the hydrogen bonds, they are included in microelectronic circuits similar to "proton networks."

It is realized microelectronic circuit in the environment CADENCE, whose output characteristics were similar to output characteristics of the hydrogen bonding networks involving water molecules. The results were compared with previously obtained results from Matlab. The hydrogen bonding network is shown on Figure 1. Figure 2 shows the microelectronic circuit with block-elements that emulate the network of Figure 1. In Figure 3 is given the microelectronic circuit that is functionally analogous to the hydrogen bonding network and it is described in Cadence.

II. CIRCUITS

The hydrogen bonding network in Figure 1 [15] shows the connections between each heavy atom.

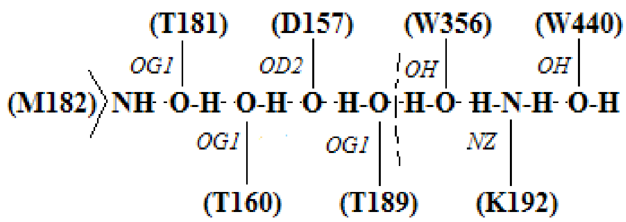

FIG. 1: HYDROGEN BONDING NETWORK IS VIRTUALLY SEPARATED INTO TWO PARTS (WITH DASHED LINE). (M182) IS METHIONINE RESIDUE, OG1 IS HYDROXYL OXYGEN OF THREONINE RESIDUES (T160, 181, 189), OD2 IS CARBOXYL OXYGEN OF ASPARTIC ACID RESIDUE (D157), NZ IS NITROGEN ATOM OF LYSINE RESIDUE (K192), OH IS OXYGEN ATOM OF WATER MOLECULES (W356, 440).

On the base of such hydrogen bonding network, the functionally analogue microelectronic circuit is developed (figure 2).

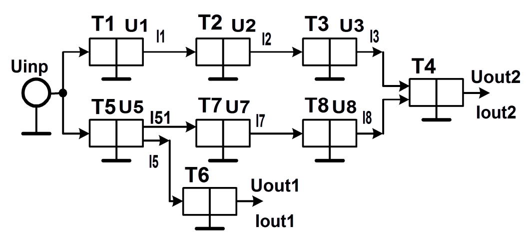

FIG. 2. MICROELECTRONIC CIRCUIT ANALOGOUS TO HYDROGEN BONDING NETWORK.

Considering the strong proton donor properties of M182N and K192NZ from figure 1, these residues can be compared to voltage controlled current sources in the analogous electrical circuit (figure 2). M182N is equivalent

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to T1 – 3-terminal block-element with one input and one output, and K192NZ is described with T5 block-element – current source with one input and two outputs. The input and output voltages of T5 are equal but its output currents have to be different because the currents depend on the specific proton transfer conditions. In the analogue microelectronic circuit all threonine residues (T160, 181, 189) are emulated by T2, T3, T8 – three-terminal block-elements and each three-terminal block-element is modeled with equal input and output voltages and different input and output currents. The block-element T4 sums the two signals. It is borrowed from D157OD2 which is strong proton acceptor. T6 and T7 emulate the water molecules W356 and W440 by 3-terminal block-elements with input and output voltages that are equal and input and output currents that are different [13].

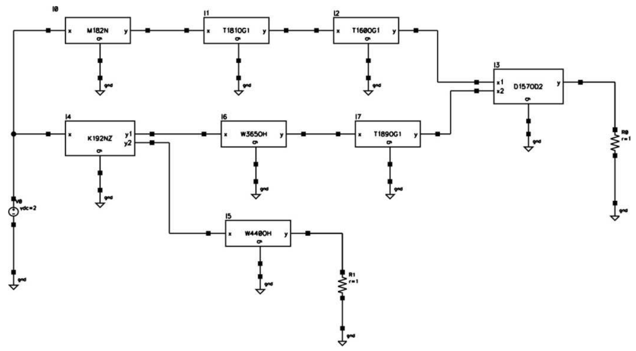


FIG. 3 CIRCUIT OF HYDROGEN BONDING NETWORK IN CADENCE.

The voltage and current relations in each block-element are described by polynomials of different orders. These polynomials are coded in Matlab and in Cadence.

Below are listed the current and voltage equations of block-element T1 describing the properties of M182N

$$U_1 = U_{in} = [-2.1:0.1:2.65]; \tag{1}$$

$$I_1 = 7.10^{-5}*U_1^4 – 7.10^{-6}*U_1^3 - 0.0011*U_1^2 +0.0047*U_1 + 0.2514; \tag{2}$$

Below are listed the current and voltage equations of block-element T2 describing the properties of T181OG1

$$U_2 = 0.974*U_1 +0.0627; \tag{3}$$

$$I_2 = -6.10^{-6}*U_2^4 - 0.00012*U_2^3 + 0.00035*U_2^2 + 0.0013*U_2 +0.0083; \tag{4}$$

Below are listed the current and voltage equations of block-element T3 describing the properties of T160OG1

$$U_3 = 1.0248*U_2 +0.028; \tag{5}$$

$$I_3=0.00019*U_3^3 -0.0003*U_3^2 -0.0021*U_3 +0.0101; \tag{6}$$

Below are listed the current and voltage equations of block-element T5 describing the properties of K192NZ

$$U_5 = 0.894*U_1 +0.2369; \tag{7}$$

$$I_5 = 0.0006*U_5^4 +0.9.10^{-5}*U_5^3 -0.0064*U_5^2 +0.0061*U_5 +0.072; \tag{8}$$

$$I_{51} = -0.0013*U_5^5 +0.0039*U_5^4 +0.0041*U_5^3 -0.016*U_5^2 +0.0045*U_5 +0.057; \tag{9}$$

Below are listed the current and voltage equations of block-element T6 describing the properties of W440OH. This block-element is the first output of the microelectronic circuit.

$$U_6 = 1.0809*U_5 +0.1706; \tag{10}$$

$$I_6 = I_5; \tag{11}$$

Below are given the current and voltage equations of block-element T7 describing the properties of W365OH

$$U_7 = 1.0004*U_5 +0.1371; \tag{12}$$

$$I_7 = 0.000495*U_7^5 -0.00207*U_7^4 -0.0013*U_7^3 +0.0116*U_7^2 -0.0006*U_7 +0.0353; \tag{13}$$

Below are given the current and voltage equations of block-element T8 describing the properties of T189OG1

$$U_8 = 0.0303*U_7^2 +0.9435*U_7 -0.3204; \tag{14}$$

$$I_8 = -6.10^{-6}*U_8^5 +10^{-5}*U_8^4 +5.10^{-5}*U_8^3 -6.10^{-5}*U_8^2 - 0.000189*U_8 +0.00064; \tag{15}$$

Below are listed the current and voltage equations of block-element T4 describing the properties of D157OD2. This block-element is the second output of the microelectronic circuit.

$$U_4 = 0.9904*U_8 +0.0967; \tag{16}$$

$$I_4 = I_3 + I_8; \tag{17}$$

Some of the block-element equations in Verilog A are given below. The rest of the equations are similar to these.

Verilog A code:

```
// VerilogA for VerilogA, 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) <+
7*10e-5*V(y)*V(y)*V(y)*V(y)-7*10e-
6*V(y)*V(y)*V(y)-
0.0011*V(y)*V(y)+0.0047*V(y)+0.2514;
end
endmodule

// VerilogA for VerilogA, W365OH, veriloga

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

module W365OH (x, y, g);
inout x, y, g;

electrical x, y, g;
electrical Vin;
analog
begin
V(Vin) <+ V(x, g);
V(y) <+ 1.0004*V(Vin)+0.1371;
I(x, y) <+
0.000495*V(y)*V(y)*V(y)*V(y)*V(y)-
0.00207*V(y)*V(y)*V(y)*V(y)-
0.0013*V(y)*V(y)*V(y)+0.0116*V(y)*V(y)-
0.0006*V(y)+0.0353;
end
endmodule

// VerilogA for VerilogA, W440OH, veriloga

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

module W440OH (x, y, g);
inout x, y, g;
```

```
electrical x, y, g;
electrical Vin;

analog
begin
V(Vin) <+ V(x, g);
V(y) <+ 1.0809*V(Vin)+0.1706;
I(x, y) <+
0.0006*V(y)*V(y)*V(y)*V(y)+0.9*10e-
5*V(y)*V(y)*V(y)-
0.0064*V(y)*V(y)+0.0061*V(y)+0.072;
end
endmodule
```

III. DC ANALYSES

DC analysis with input voltage between -2.1 and +2.65 [V] is performed. The output characteristics of the microelectronic circuit I_{out1}, $I_{out2} = f(U_{in})$ (figure 4 Matlab and figure 5 Cadence) are similar with the output characteristics of differential amplifier [16]. When the input voltage increase the output current of first output decrease, while the current output of the second output increase. Both output currents are positive all the time and they saturated. We can see different between this circuit and classic amplifier, here output current change them values in different intervals (they are shift from each other). This is true for both simulations – in Matlab and in Cadence.

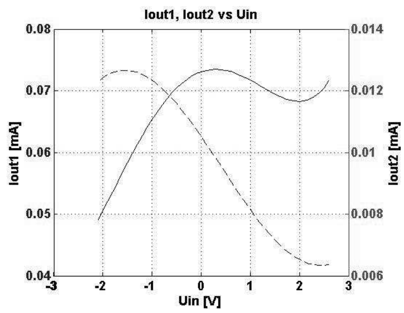
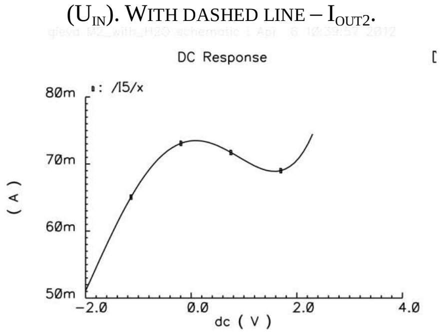
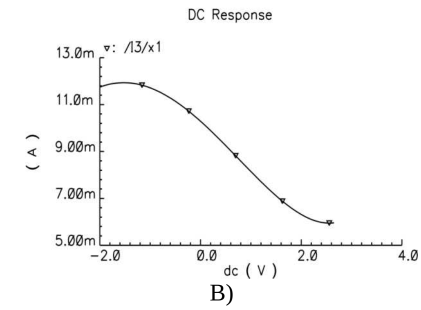


FIG. 4 OUTPUT CURRENTS (I_{OUT1} AND I_{OUT2}) VS. INPUT VOLTAGE (U_{IN}). WITH DASHED LINE – I_{OUT2}.



A)



B)

FIG. 5 OUTPUT CURRENTS (A)I_{OUT1} AND B)I_{OUT2}) VS. INPUT VOLTAGE.

The voltage transfer characteristics (figure 6) show that both output voltages are linear functions of the input voltage and are shifted to each other. Hence, the microelectronics circuit analogous to the HBN with water molecules and protein residues could operate as CMOS differential power amplifier.

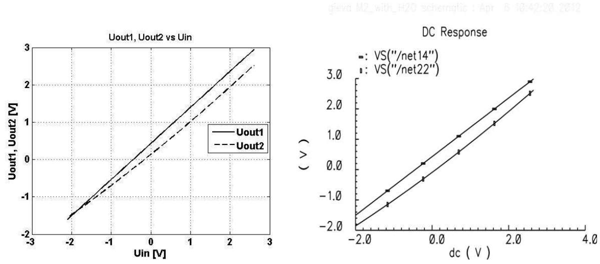


FIG. 6 OUTPUT VOLTAGES (U_{OUT1} AND U_{OUT2}) VS. INPUT VOLTAGE (U_{IN}) A) MATLAB AND B) CADENCE.

IV. TRANSIENT ANALYSES

The transient analysis is performed with two different input voltages – figure 7 and figure 10. First is applied input voltage from figure 7 with amplitude from -2.4 to +2.4 [V] and frequency 10 [GHz].

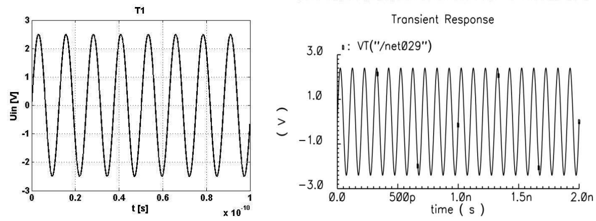


FIG. 7. INPUT VOLTAGE (U_{IN}) VS. TIME (T).

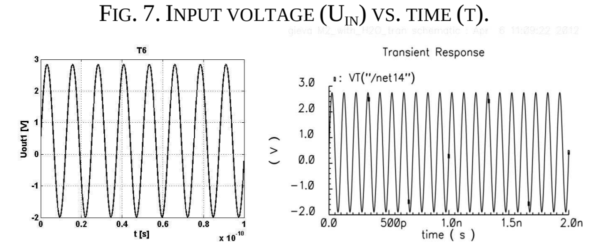


FIG. 8. FIRST OUTPUT VOLTAGE (U_{OUT1}) VS. TIME (T).

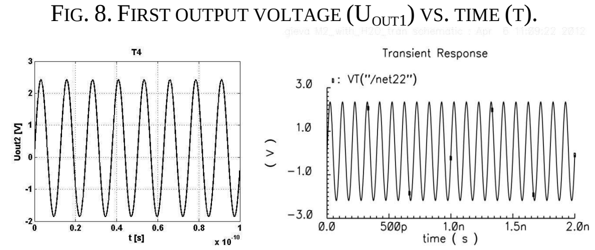


FIG. 9. SECOND OUTPUT VOLTAGE (U_{OUT2}) VS. TIME (T).

When is applied input voltage from figure 7 we can see the follow results for outputs voltages on figure 8 (for first output) and on figure 9 (for second output) in Matlab and in Cadence. The results in all outputs from both simulation are identical. There is not differences.

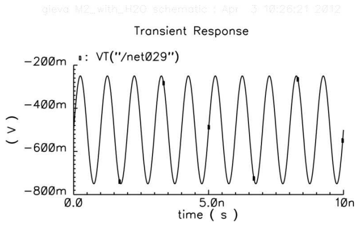


FIG. 10 NEGATIVE INPUT VOLTAGE (U_{IN}) VS. TIME (T).

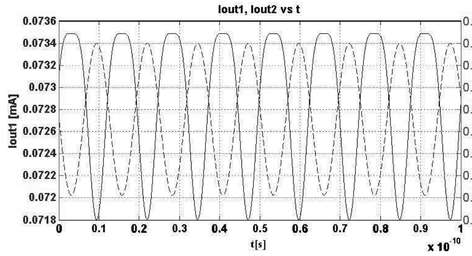
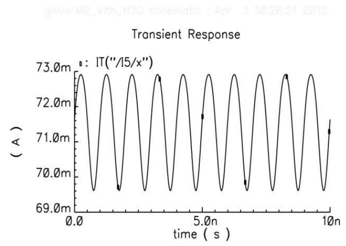
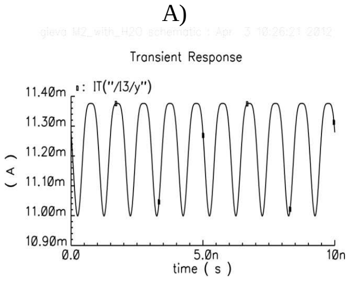


FIG. 11 OUTPUT CURRENTS (I_{OUT1} AND I_{OUT2}) VS. TIME (T). WITH DASHED LINE – I_{OUT2} IN MATLAB.



A)



B)

FIG. 12. OUTPUT CURRENTS (A) I_{OUT1} AND B) I_{OUT2}) VS. TIME (T) IN CADENCE.

When was applied input voltage of figure 10 have the following results in the outputs that were shown on figure 11 and figure 12. Considering the results in output in both environments (Matlab and Cadence) we see that the curves have identical shape, phase and they are positive when is applied negative input voltage. Difference was observed in the amplitude and range of the signal. The results from Cadence have higher values. Previous tests have shown that the amplitude of input voltage over 0,3 [V] occurs first signal distortion in one channel and then in the other. That's way we applied two different input voltages. The circuit work stabel when is applied negative input voltages from figure 10.

V.CONCLUSION

The analysis shows that the output voltages repeat input and therefore remain sinusoidal waveform. Typically currents of output channels is that the negative half period of input voltage, the two sinusoidal currents are positive. The current of the first channel is in phase with the output voltage until the current of the second channel is in antiphase. Therefore, this circuit could work as a generator of alternating-current signal, CMOS power amplifier or differential amplifier. Hydrogen bonding network is one very promising and suitable objects for development of future electronic devices.

VI. ACKNOWLEDGEMENTS

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