From Layout to System Simulation: An Example of an Oxygen Sensor

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ABSTRACT

The development of microsystems has shown that the technologies and tools are mature enough to investigate the possibilities of complete CAD tools, as is the case in integrated circuit design. An oxygen sensor has been taken as an example. A parametrized cell has been created within the CADENCE framework allowing the layout design of the structure without knowledge of the technologies. On the other hand, the model has been implemented in the MAST analog hardware description language taking into account the diffusion effect. This model can be associated with other electric components of the system in the SABER software simulator to predict the behaviour of the system or to optimize the sensor geometry.

Keywords: layout, chemical sensor, diffusion, system simulation

INTRODUCTION

Some examples have been developed demonstrating the possibility to go from the layout level to the system simulation level. Design kits have been already proposed for technologies like CMOS [1, 2] and SIMOX [private communication]. However, these tools are not adapted to the technological process of an oxygen gas sensor presented in this paper. Thereby, we have developed a dedicated parametrized cell and its associated model that will allowed simulating the sensor with other components of the data processing system.

OXYGEN SENSOR DESCRIPTION

Sensing Principle

The oxygen sensor [3] is a miniaturized Hersch battery. This electrochemical cell consists of two electrodes: the working electrode made of gold and the counter electrode made of lead. These electrodes are immersed in a liquid electrolyte and the whole is separated from the solution to be tested by a porous membrane.

After diffusion through the membrane and the electrolyte, the oxygen molecules are reduced at the working electrode:

$$O_2 + 2H_2O + 4e^- \text{ -------> } 4OH^-$$

and the counter electrode is oxidized following the reaction:

$$Pb + 2OH^- \text{ -------> } PbO + 2e^- + H_2O$$

The main advantage of this sensor is that no external polarization is needed: the electrochemical potential of electrode materials is such that the working electrode is naturally set to the oxygen reduction potential. This sensor is thus less sensitive to interfering species and electrical variations.

Description of the device

The device is made of two micromachined silicon wafers. A schematic cross-sectional view is given on figure 1 and a top view is given on figure 2. The lower wafer supports the active part

- the gold electrode is deposited by an evaporation process. To improve the adhesion of gold on to the silicon, a NiCr layer is deposited on the silicon before the gold film
- the lead electrode is obtained by electrochemical deposition. The lead layer is typically 10 µm thick
- the cavity that will contain the electrolyte is obtained by anisotropic KOH etching of the silicon wafer.

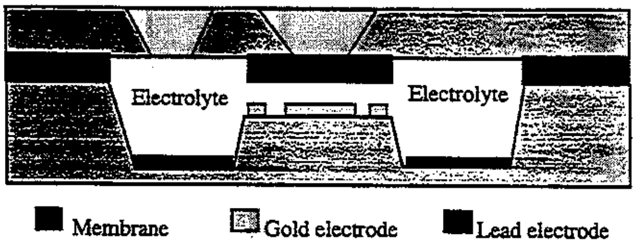

Figure 1. Cross sectional view of the O_2 sensor

The upper part supports the porous membrane.

Two holes are first micromachined by chemical etching of silicon. One of them will be covered by the membrane and will allow the contact between the active area and the solution to be tested. The other one will be useful to fill up the cavity with the electrolyte. The membrane is a silicon paste spun and thermally polymerized on to the silicon wafer.

The two parts are assembled and the cavity is finally filled, just before utilisation.

All the silicon substrates are coated with a Si_3N_4 layer in order to insulate the electrode from the substrate to prevent leakage current and to protect silicon from chemical etching.

The general specifications of the sensor are presented in the following table.

Table 1. Specifications of the sensor

Sensibility:	10 pA/ppb
Range of detection:	0 to 20000 ppb
Working temperature:	0 to 60 °C
Life time:	1 year
time:	< 1min

These specifications lead to the following and dimensions. The surfaces of the working and lectrode are respectively 0.09 mm^2 and 80 mm^2 olume of electrolyte contained in the cavity is 10

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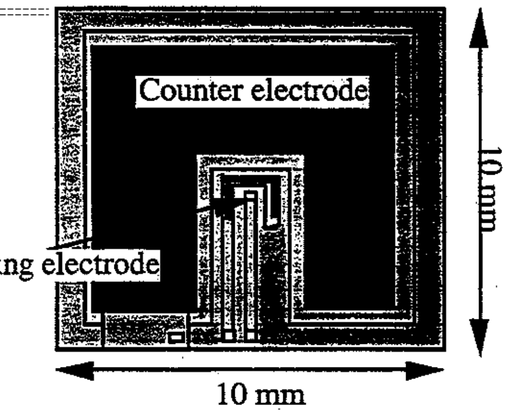

gure 2. General view of the oxygen sensor

LING OF THE SENSOR BEHAVIOR

As we have seen previously, the oxygen s diffuse through the membrane and then through rolyte before reaching the electrode. As the emical reactions are fast compared to the process, the response time of the sensor will thus ainly on the diffusion through both electrolyte orane. The current can be expressed as [4]:

$$S D_i \left[\frac{\partial C}{\partial x}\right]_{L_m}^{L_e} \qquad (1)$$

is the number of electrons involved in the emical reaction, D_i the diffusion coefficient of the material i, S the working electrode surface and F the Faraday constant, L_e the electrolyte thickness and L_m the membrane thickness. The time diffusion through the membrane and electrolyte is thus:

$$t = \frac{L_e^2}{k^2 D_e} + \frac{L_m^2}{k^2 D_m} \qquad (2)$$

where the index e and m denote respectively electrolyte and membrane and k is the distribution coefficient.

The value of the coefficient D_e is $D_e = 10^{-5}$ $cm^2.s^{-1}$ and the corresponding response time t_e, for a 10 µm thick electrolyte is in the range of 1 ms. The value of t_m is around several hundred times larger for available membrane materials. As a consequence the diffusion trough the electrolyte will be neglected and the diffusion phenomenon will be described by the Fick equation:

$$\frac{\partial C(x,t)}{\partial t} = D_m \frac{\partial^2 C(x,t)}{\partial x^2} \qquad (3)$$

In the case of an oxygen step, this equation can be solved analytically and the current can be written as follow:

$$I(t) = I_{stat}\left(1 + 2\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{n^2\pi^2 D_m t}{L_m^2}\right]\right) \qquad (4)$$

With I_{stat}, the current in the steady state.

$$I_{stat} = N F S \frac{P_m}{L_m} C_s \qquad (5)$$

N, the number of electrons involved in the chemical reaction; F, the Faraday's constant; S, the surface of the working electrode; P_m,D_m and L_m the diffusion coefficient, permeability and thickness of the membrane and Cs the oxygen concentration.

All input shapes can be approximated by a combination of steps and, because this differential equation is linear, the output can be easily calculated.

PARAMETRIZED CELL

As for electronic components, a library is composed of elements subject to the same design rules. The parametrized cell was developed within the CADENCE framework. It is designed with the Virtuoso Layout Editor and the design rules are automatically checked with a DRC (Design Rule Checking) program under DIVA. The compiled layout can be converted in a format readable by a mask generator. An extracted view can be generated to verify the electric connection by comparison between the physical connection at layout level and its schematic representation.

Because of the specificity of the process flow chart, a technological file was created.

Limitations and design rules

Limitations of oxygen sensor layers on layouts are imposed by the used technological steps and the capacity of the lithographic process. Regarding the final dimensions of the sensor, we have considered that a minimal size of five microns is enough resulting in the two following rules: all widths have to be bigger than fives microns and two patterns have to be separated by a minimum of five microns.

Following the process flow chart described above, the realization of the lower part of the oxygen sensor is obtained by two anisotropic wet etching : one for the electrolyte tank (layer "Tank", mask N° 1) and the second for the central part under the membrane (layer "Central_Gap, mask N°2). This last thickness will define the response time of the diffusion phenomena through the electrolyte. It is adapted in order to be negligible in regard of the response time induced by the membrane itself that can not be chosen by the user. The final 3D form obtained with such chemical process is defined by the <111> oriented planes with an angle of 54,7° with the substrate surface in the case of concave corners, and by the fastest planes for convex corners. A first consequence, to respect the final surface of the counter electrode, and so the estimated lifetime of the oxygen sensor, is that masks corresponding to the "Tank" and the "Central_Gap" have to be larger. The modification between the effective surface and the mask geometry is automatically calculated and taken into account. A second aspect is the underetching at convex corners surrounding the central part inside the tank. Instead of creating compensation structures, a one hundred microns gap between the layer "Poly" and the layer "Tank" and a fifty microns gap between the layer "Poly" and the layer "Central_Gap" are introduced. Otherwise no modification due to optical reasons have to be taken into account because of the geometry of the tank (thickness around one hundred microns, wavelength of 450 nanometer).

Parametrical cell inputs

We have defined a set of geometrical parameters to design an adapted layout of the structures. These geometrical parameters play a role in the behaviour of the oxygen sensor and can be modified through the window "Edit Instance Properties". We have allowed the users to modify dimensions of: the working electrode (ET_x, ET_y), the ring belt (e_x_l, e_x_r, e_y),(see figure 3), the counter electrode (CE_x_l, CE_x_r, CE_y) (see figure 4) and pads sizes. The pad sizes in order to allow different bounding techniques. The counter electrode surface is related with the lifetime of the sensor. The surface of the work electrode influences proportionally the static current delivered. The ring belt avoids the oxygen, included in the electrolyte after different measurement sequences, to participate to the current and so to induce an error. Experiments have shown that the best fit is when the two surfaces are equal. To insure this last aspect, dimensions have to respect some relations. The figure 6 shows the window of a parametrical cell and the layout modification parameter window.

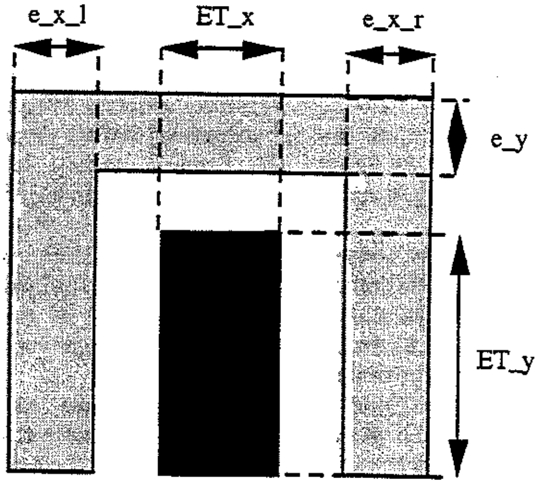

Figure 3. Schematic of working electrode and ring belt

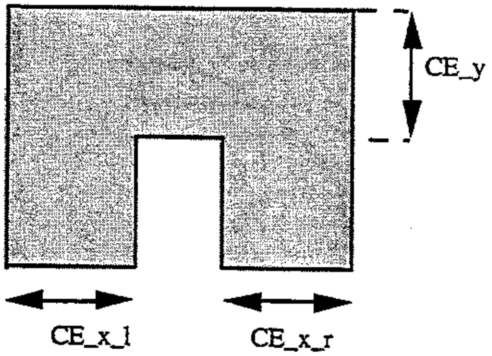

Figure 4. Schematic of counter electrode

Grading of structures

Inside a library, it is possible to combine basic cells to create larger structures. Basic cells are imported with their properties as "instance" in a new layout type structure. Depending on cell sizes, their location can be optimized on a wafer. As specified in the process description, the lead deposition to form the counter electrode is obtained by electrodeposition. Each counter electrode has to be connected together depending on location on the wafer with enough space between each cell for sawing step. This procedure is automatic and an example with eight oxygen cells is shown on figure 7. At the same time, the mask for the upper wafer is generated with respect to working electrode surface and location on the wafer.

SYSTEM SIMULATION

One goal of the study presented in this paper is to demonstrate the possibilities to optimize the conception of chemical sensor and its associated processing electronic by the way of simulation. This approach needs to be able to simulate the sensor in its electronic environment, and to describe interactions between layout parameters like dimensions, and parameters used in simulations.

Today, simulation tools like ELDO, SABER, .. are able to associate components from different domains in the same simulation. But the component library proposed by this tools does not include chemical devices. So, the first step of our work has been to write a model of the oxygen sensor.

The tool chosen for this application is the analog and mixed-mode simulator form ANALOGY : SABER. Its open architecture allows the users to create new models form scratch in C, Pascal, Fortran or in Analogy's analog hardware descriptive language named MAST.

The oxygen sensor model is based on the analytical solution of the diffusion equation after a step of the oxygen concentration (equation 4). Nevertheless, we have extended it to any kind of input by using step decompositions (figure 5).

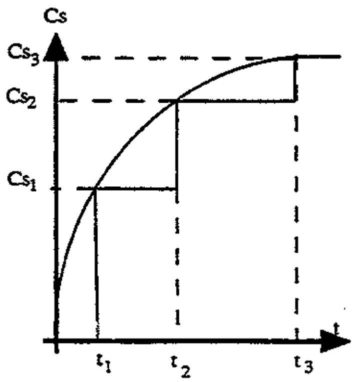

Figure 5. Step approximation of the input.

Then, the current delivered by the sensor can be approximate by:

$$I(t) = a\sum_{k}\left(1+2\sum_{n=1}^{\infty}(-1)^{n}\exp[b(t-t_{k})]\right)(C_{S_k}-C_{S_{k-1}}) \quad (6)$$

$$\text{with: } a = NFS\frac{P_m}{L_m} \quad b = \frac{n^2\pi^2 D_m}{L_m^2}.$$

The SABER model of the oxygen sensor has been written in C, because the loop instruction necessary to implement equation 6 is not available in the MAST language

Figure 8 shows the schematic of the circuit implemented in SABER simulator to validate the oxygen sensor model. Figure 9 represents the behaviour of this model when the oxygen concentration varies.

The geometrical parameters of the parametrized cell are near to be transferred automatically to the SABER model We also plan to develop an interface, which allows to transmit modifications of parameters in SABER to the CADENCE layout tool, in order to verify these modifications are fulfil design rules of the technology.

CONCLUSION

In this paper, we have presented an example of the conception of an oxygen sensor from layout to system simulation. A specific technology file has been created within a Cadence framework including specific processes like anisotropic chemical etching and electrodeposition. The design rules checking is included allowing a conception without specific knowledge of the technological flow chart.

We have chosen a system simulator named SABER because it permits to associate physical models with an electrical environment.

The conception of sensing cell and the associated electronic environment can be made simultaneously. The user can optimise the electronic in regard with layout sizes of the sensor or optimise the layout in regard of the electronic environment. The next point to be include in this work is the generation of parasitic elements

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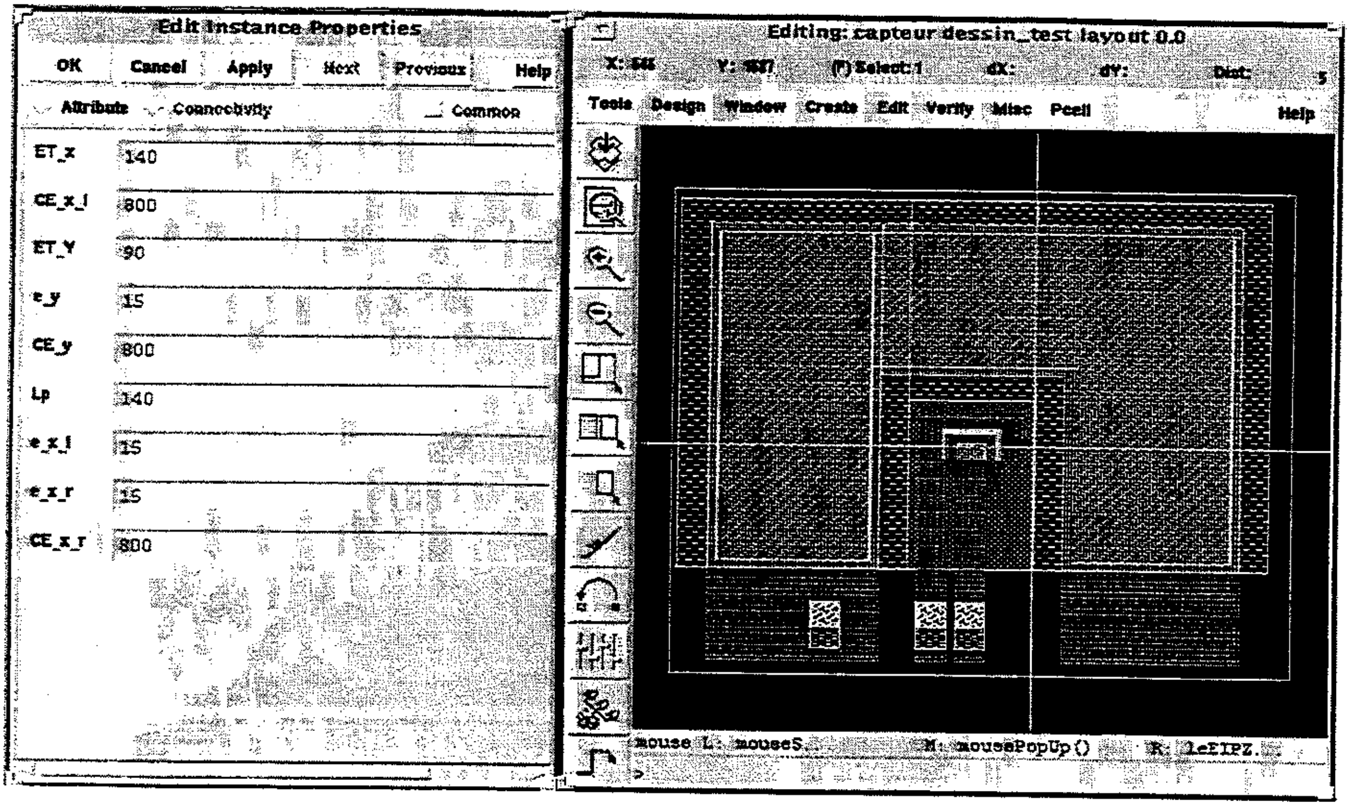

ET_x 140

CE_x_l 800

ET_Y 90

e_y 15

CE_y 800

Lp 140

e_x_l 15

e_x_r 15

CE_x_r 800

Figure 6. Layout of the parametrised cell and instance properties window

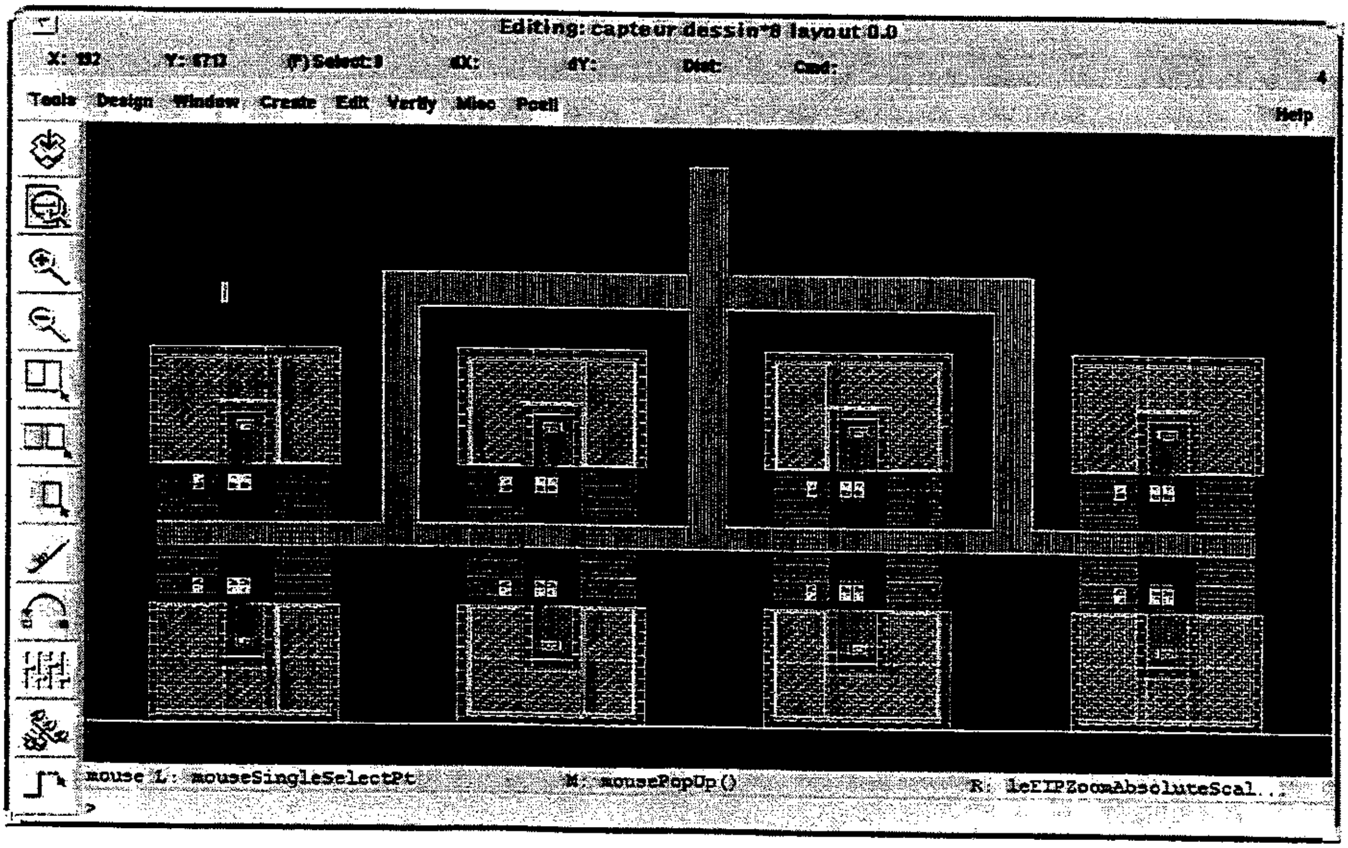

Figure 7. Automatic location of sensing on a wafer with connection for electrodeposition

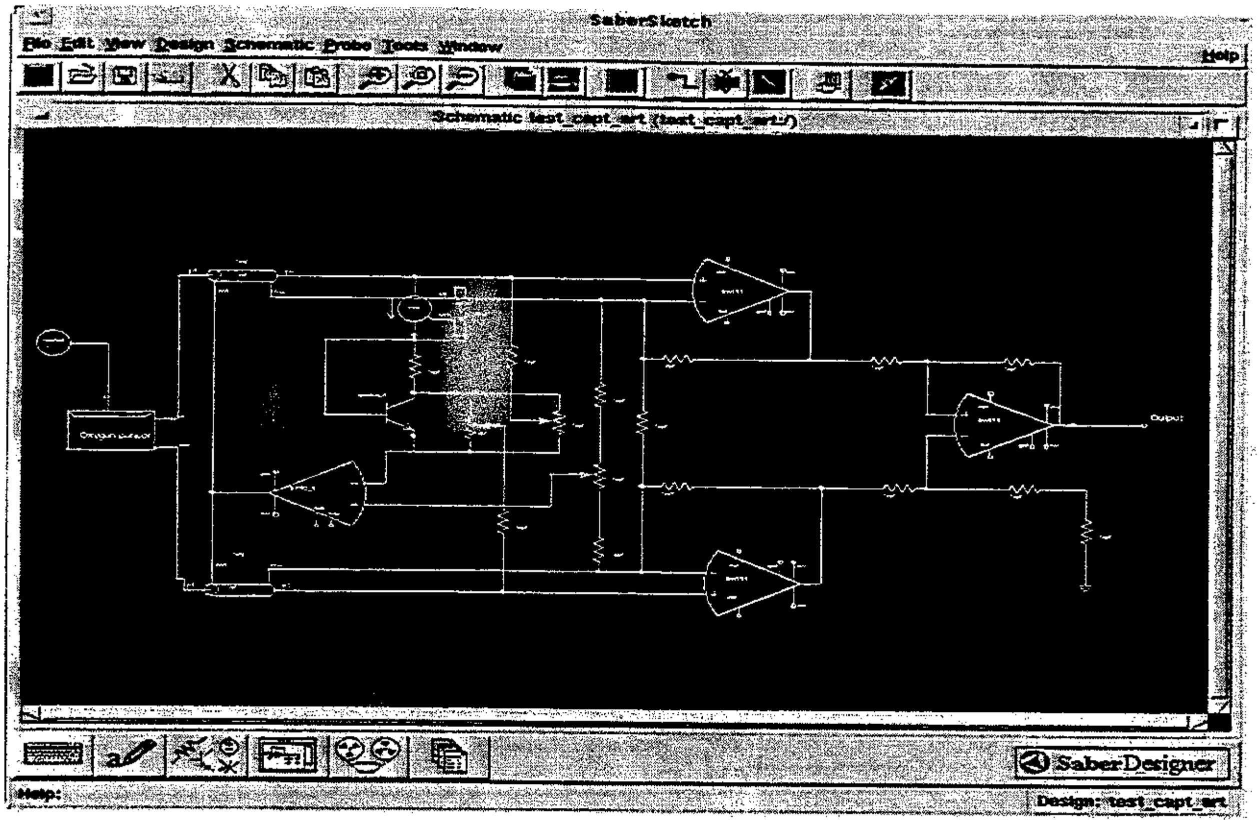

Figure 8. Schematic of the circuit implemented in SABER simulator.

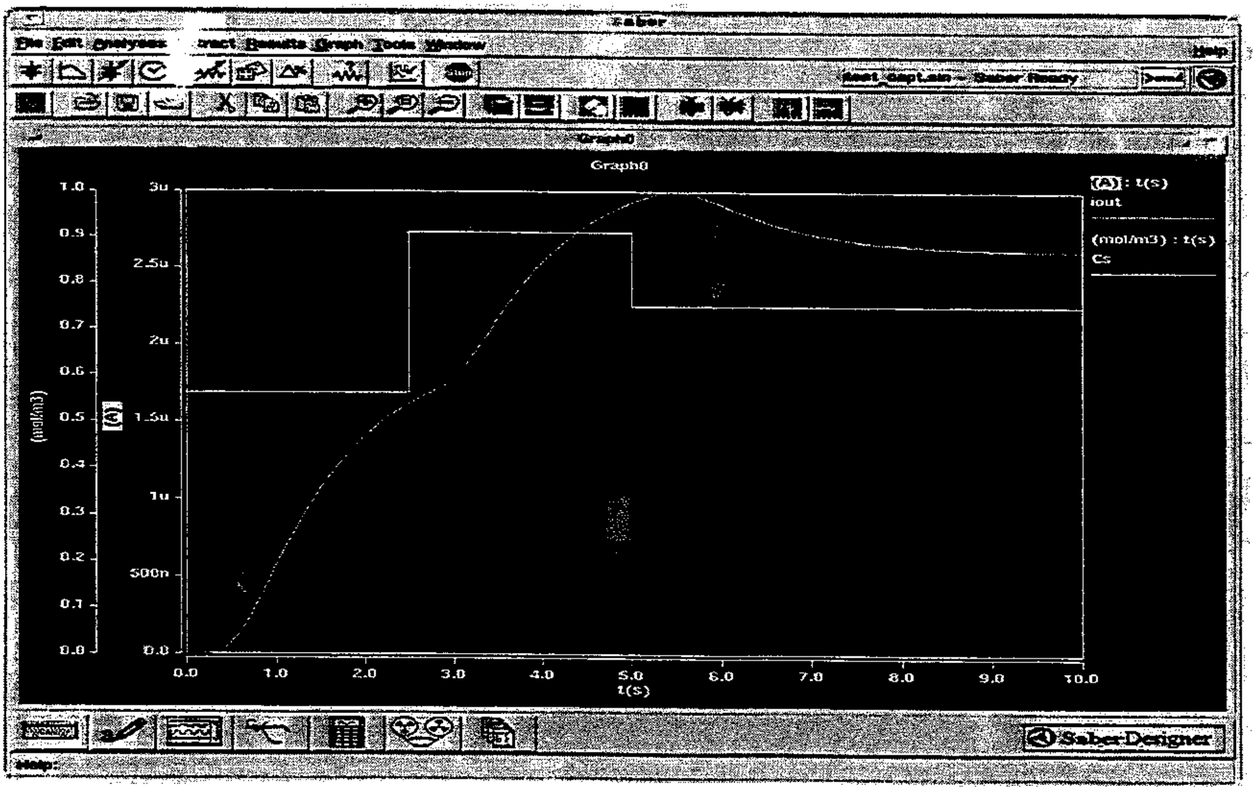

Figure 9. Response of the output current when oxygen concentration varies.