PSPICE model for resistive gas and odour sensors

J.W.Gardner, E.Llobet and E.L.Hines

Abstract: A generalised PSPICE model of resistive gas/odour sensors is presented. The model simulates the response of both polymeric and metal oxide devices, as well as an integrated resistive heater that is used to set the operating temperature. In both cases there was good agreement between the observed responses and the PSPICE simulated responses to rectangular pulses of gases. The PSPICE model is not only simpler and faster to use than analytical solutions, but also should permit the rapid prototyping of associated drive circuitry.

1 Introduction

A considerable range of metal oxide films and conducting polymer films are sensitive to gases and are being used in solid-state gas sensors and electronic noses [1]. Recently developed parametric models of their transient response should help in the design of new devices and in the interpretation of experimental data [2, 3]. Moreover, their dynamic response has been shown to contain useful information for improved gas recognition [4]. The PSPICE program is a widely used CAD program to construct models of electronic devices, and to simulate linear and nonlinear circuitry [5, 6]. A mathematical model of a device may be constructed either from observed input–output data or from a physical model. Although an exact analytical model is based on the physical and chemical properties of the sensing material and provides some insight into the sensor behaviour, a PSPICE behavioural model has the advantages of being easier to construct and implement. Furthermore, existing PSPICE modules (such as noise or Monte Carlo analysis) make this tool both versatile and flexible for the study, characterisation and optimisation of gas sensors within a measurement circuit. The availability of SPICE models is growing, but until now there has been no SPICE model for either the static or dynamic response of gas (or odour) resistive sensors. In this paper we report on the use of PSPICE to construct a generic model that simulates the behaviour of both metal oxide and conducting polymer resistive gas sensors. The modelling strategy is based on detailed theoretical and experimental analyses reported elsewhere [2–4].

2 PSPICE model description

First, a brief description is given of the typical response of a resistive sensor to gas pulses. The precise mechanisms of the interaction between the active film and the gas molecules, and the manner in which these generate a change in the electrical resistance of the film, remain the subject of research. Previously developed analytical models [2, 3] consider the adsorption and/or reaction of the gas molecules onto active sites distributed in the sensing material. There is experimental evidence [3, 7–9] to suggest that the static response (i.e. conductance G, of these devices) follows a simple, reversible, binding isotherm.

For metal oxides:

$$G = G_0 + aC^r \qquad \text{(Freundlich isotherm)} \qquad (1)$$

For conducting polymers:

$$G = G_0 + a\frac{bC}{(1+bC)} \qquad \text{(Langmuir isotherm)} \qquad (2)$$

where C is the maximum concentration of the gas pulses, G_0 is the base-line conductance of the device in air, a is a sensitivity coefficient, r the power law exponent for oxides and b the binding constant for polymers. Recent work has resulted in the introduction of dynamic models in which the gas is assumed to diffuse into the sensing film and is, simultaneously, adsorbed at fixed sites distributed throughout the film. The time dependence of the conductance of the sensing device is then calculated and related to the device geometry and rate kinetics [2, 3]. Fig. 1 shows some typical transient responses for resistive gas/odour sensors. It can be seen that the sensor responses appear to be characteristic of a first- or a second-order system.

Both the static and transient responses depend strongly on the operating temperature T of the sensor. Whilst metal oxide sensors operate at high temperatures of c. 400°C, conducting polymer sensors operate close to room temperature (e.g. 40°C). Both types of sensor usually possess an integrated resistive heating element that can be used to set their precise operating temperature above ambient conditions.

The PSPICE model shown in Fig. 2 mimics the behaviour of metal oxide and conducting polymer gas sensors. Its main features are as follows:

- A voltage source is used to emulate the input of gas pulses in which the voltage is equivalent to the gas concentration (C). Gas pulses allow the adsorption (ON) and desorption (OFF) profiles of the device to be simulated.
- A nonlinear analogue behavioural model (ABM) block performs either a Freundlich (metal oxides) or a Langmuir (conducting polymers) transformation of the gas pulses.

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J.W.Gardner and E.L.Hines are with the School of Engineering, University of Warwick, Coventry CV4 7AL, UK

E.Llobet is with Departament d'Enginyeria Electronica, Universitat Rovira i Virgili, Autovia de Salou s/n, 43006 Tarragona, Spain

This block simulates the static gain or sensitivity of the device.

- The transformed signal is fed into two parallel-connected unity gain low-pass filters, which are used to model the transient behaviour of the sensors. Earlier work suggests that the response of resistive gas sensors may be described by a second-order multi-exponential model [10]. Therefore, in our PSPICE model the ON and OFF transients are simulated by second order low-pass filters, whose transfer functions can be written as:

$$H(s) = \frac{A}{(1+as)(1+bs)} \tag{3}$$

where A, a and b are real parameters because, if the imaginary part of a and b were non-zero, the transient response would show oscillations, which is clearly not the case (see Fig. 1).

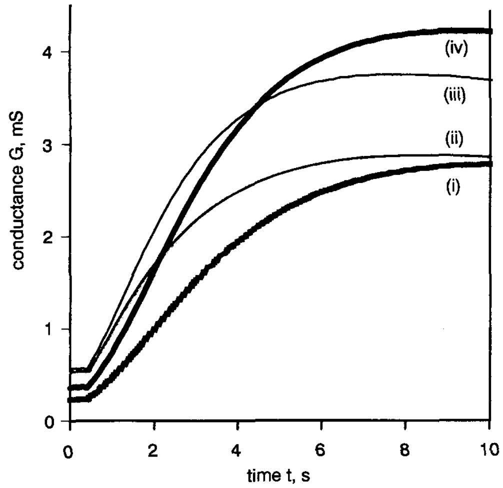

Fig. 1 *Typical transient responses of four solid-state gas sensors to odour pulse*
(i) Sensor 1; (ii) sensor 2; (iii) sensor 3; (iv) sensor 4

Two different filters are required since the OFF dynamics are, in general, slower than the ON dynamics. The outputs of the filters are connected to an ABM block, which acts as a logic switch selecting the appropriate filter output (ON or OFF transient). The model switches between the two filters according to the length of the odour pulses, which is set by the user. The ABM block that acts as a switch does not make the switching effective until the output voltages of the two filters F_{ON} and F_{OFF} are equal. This avoids the occurrence of a sharp change in the voltage at the output, should the user not wait until the steady-state response before switching.

- Another ABM block acts as a voltage-controlled current source whose transconductance simulates the electrical conductance of the sensor.

The overall model can be represented as a three-pin device subcircuit, which simulates the behaviour of a gas-sensitive resistor. Fig. 2 shows a typical measuring circuit.

Our PSPICE model has been extended further both to consider the effect of a multicomponent mixture of gases and to take the device temperature into account. The case of a binary mixture is modelled by duplicating the elements inside the dashed rectangle in Fig. 2 and adding the contributions of each branch at the input of the voltage-controlled current source. This makes it possible to compute the device's response to a gas in the presence of interfering species. An additive model of conductance for the gases present in a multicomponent mixture requires that the sensor's response to each gas is unaffected by the other gases [11, 12]. This has been shown to be the case at low concentrations (up to 100ppm) for binary mixtures of volatile organic compounds [13]. The effect of the operating temperature on the sensor response is included by either using a function or look-up table for the physical parameters (e.g. sensitivity, baseline and pole positions). An ABM block emulates the heating element and sets the device operating temperature according to the approximate expression:

$$T_{device} = T_{ambient} + \alpha\left(\sqrt{1+\beta V_h^2} - 1\right) \tag{4}$$

Where T_{device} is the operating temperature of the device, V_h is the heater voltage, α and β are two device-specific coefficients relating to conductive and convective heat losses. Our strategy is flexible and makes it possible to customise the model to a particular design of device (via a change in the value of these coefficients).

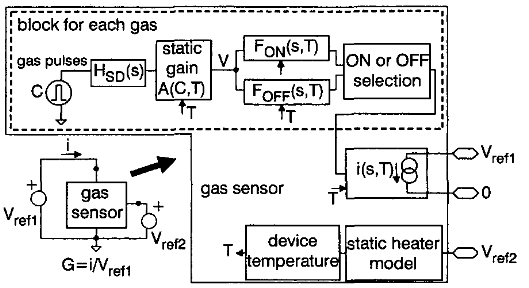

Fig. 2 *Simplified PSPICE model of resistive gas sensor as three-terminal device, and application circuit employing reference voltages for measurement and setting of operating temperature (bottom left)*

Finally, for practical implementation, the sensors are modelled to operate within a real gas flow system. Since it is almost impossible to create perfect gas pulses, a model for the sample delivery system has also been provided (see transfer function $H_{SD}(s)$ in Fig. 2). The objective of this block is to modify the shape of the gas pulses to account for experimental variation (NB this block can be disabled by the user in setting $H_{SD}(s)$ to 1). From all of the above, the dynamic conductance (ignoring constant baseline value) of the device in the Laplace domain $\tilde{G}(s, T)$ can be expressed as follows (case of a single gas):

$$\tilde{G}_{ON}(s,T) = F_{ON}(s,T)\cdot\tilde{V}(s,C,T) \quad \text{ON} \tag{5}$$

$$\tilde{G}_{OFF}(s,T) = F_{OFF}(s,T)\cdot\tilde{V}(s,C,T) \quad \text{OFF} \tag{6}$$

where T is the device temperature set by V_{ref1} and adjusts various model parameters, C is the height of the gas/odour concentration pulse, F is a transfer function for ON/OFF transients, and $\tilde{V}(s, C, T)$ is the Laplace transform of the voltage signal at the output of the static gain block (i.e. $\pm A(C, T)H_{SD}(s)U(s)$ for an input $U(s)$; see Fig. 2). A description of the model parameters for the single gas case is given in Table 1.

3 Simulation results

To check the validity of the PSPICE model, it was used to simulate the conductance transient responses of both metal oxide and conducting polymer sensors to rectangular gas pulses. Fig. 3 compares PSPICE results with transients obtained from the numerical solution of the equations of

Table 1: Parameters in the model whose values are set by the user

Parameter	Meaning
Conc_val	gas concentration
V_h	heating resistor voltage (sets operating temperature)
am_temp	room temperature
α, β	coefficients of the resistive heater empirical model
r_val	Freundlich exponent (metal oxides)
b_val	Langmuir binding constant (conducting polymers)
base	baseline sensor conductance (in air)
sens	sensitivity
f_pon	first pole low-pass filter (ON transient)
s_pon	second pole low-pass filter (ON transient)
f_poff	first pole low-pass filter (OFF transient)
s_poff	second pole low-pass filter (OFF transient)
T_on	duration of the ON pulse (gas conc. = conc_val)
T_off	duration of the OFF pulse (gas conc. = 0)
delay	delay before the first gas pulse
smooth	characterises the sample delivery system (SDS)
sds_en	set to 1 enables the SDS; set to 0 disables the SDS

our analytical diffusion-reaction model [2, 3]. The PSPICE model leads to equivalent results in less than one minute (i.e. up to ten times faster than solving numerically a diffusion-reaction model for metal oxide sensors on the same PC platform).

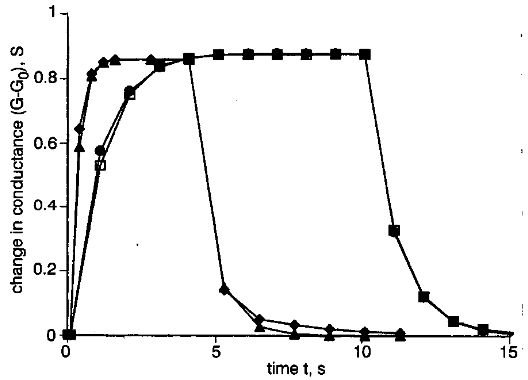

Fig. 3 *Conductance transient responses obtained using diffusion-reaction model (analytical), and PSPICE model (SPICE) of metal oxide (MOS) and conducting polymer (CP) gas sensors*
—◆— MOS, analytical
—▲— MOS, SPICE
—●— CP, analytical
—□— CP, SPICE

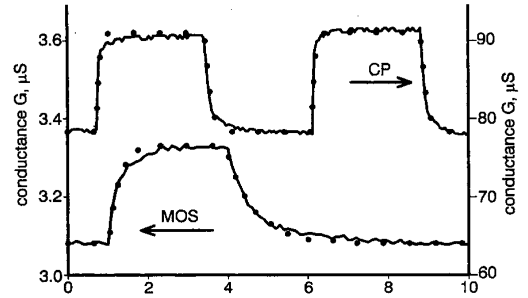

Fig. 4 *Comparison between experimental (exp), and simulated (SPICE), conductance transient responses, of poly(pyrrole) (labelled CP) gas sensor to CO_2 (right axis) and tin oxide (labelled MOS) gas sensor to CO (left axis)*
—— exp
—•—•— SPICE

Fig. 4 shows experimental transients and their simulated counterparts using PSPICE. Pulses of 10ppm (volume of gas/volume of test chamber) of CO_2 were measured using a poly(pyrrole) polymer coated sensor. The effect of drift is noticeable in the sensor response (i.e. the baseline conductance decreases and sensitivity increases with time). Pulses of 10ppm CO_2 were measured using a tin oxide gas sensor. The sensor response is less affected by drift, and the model accurately depicts baseline, steady-state responses and both ON and OFF transients. The discrepancies that exist between the experimental and the simulated transients in Fig. 4 are not significant. The most useful information (e.g. to perform gas/odour analysis) is in the steady-state response and in the part of the transient response that shows a sharp variation in conductance [4, 13]. In both cases there is an excellent agreement between the SPICE prediction and the experimental behaviour.

To set the values of the parameters in the SPICE model, it is worth using the strategy that follows:

- Parameters that define the measurement to be simulated, such as the duration of the odour pulses, the concentration, heating voltage and room temperature can be set easily by the user for each specific case.
- Parameters that characterise the sample delivery system only need to be found the first time and then can be stored for future use. This is also true for the parameters of the empirical heater model.
- Finally, the values of the parameters that characterise the static and transient responses of the sensor need to be adjusted by a trial and error procedure. However, these parameters can be estimated by performing measurements with real sensors.

Finally, Fig. 5 shows a simulated response of a metal oxide sensor for two different operating temperatures 350°C and 240°C (V_h set to 6.0V and 3.0V, respectively). Sensitivity, baseline and dynamics can all vary with the operating temperature of the device.

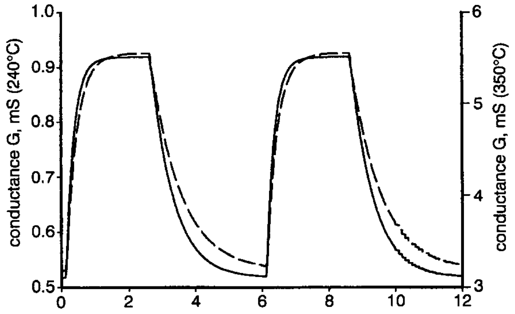

Fig. 5 *Effects of varying temperature of operation of metal oxide device*
---- 240°C
—— 350°C

4 Conclusions

Metal oxide and polymer resistive gas sensors are widely used and yet their exact sensing mechanisms are complex and still the focus of research. Therefore, strategies to model their response based on behavioural descriptions may be very helpful to end-users. In this context, SPICE models for the static and transient response of resistive gas sensors have been reported for the first time. PSPICE is shown here to be useful in synthesising behavioural models of resistive gas sensors. Our model is applied here to predict the effect of multicomponent gas mixtures and operating temperature, but it can easily be extended to cover other types of device, such as capacitive or gravimetric. (The PSPICE dynamic models of resistive gas sensors described here are available from the authors on request.)

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