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# Thermal Simulation and Package Investigation of Wireless Gas Sensors Microsystems

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**Abstract:** Gas sensor arrays based on metal oxides operating at high temperature are commonly used in many application fields. They can operate on different principles and each sensor may show very different responses to the individual gases in the environment. Data coming from the array can be merged for reliable gas detection. One point which is common to the different sensors types is that the atmosphere to be sensed must flow on or through the sensor itself. This work investigates air flows in gas sensor packages, and proposes a new package to improve gas exchange through natural convection, aiming to allow the gas detection in the case of very small gas concentrations. The study is based on multiphysics Finite Element Method simulations using Comsol predefined equations.

**Keywords:** sensor package, free convection, air flow, heat transport, mass transport.

## 1. Introduction

Gas sensors can be used in several applications like standard fire alarm, Wireless Sensor Networks and monitoring environmental conditions [7] [8]. As chemical gas sensors are based on chemical reactions between the sensor itself and the molecules of the analyzed gas, the detection of gas is possible only if the desired molecule comes in contact with the sensing material [1]. This is why the package of a gas sensor needs apertures to let the gases enter and react with the sensing elements. However, to avoid damages to the sensor, it is necessary to eliminate the particles and relatively big objects by filtering the air entering into the sensor.

The transport of a passive tracer in the atmosphere may occur either through molecular diffusion from the higher concentration zone to the lower concentration zone and/or by advection by the air flow. The latter process is much faster than diffusion and needs to be optimized to achieve a higher sensor's efficiency by increasing the probability of gas molecules impact on the sensor's surface per unit time.

Chemical gas sensors work at high temperature (typically around 300-400°C) which triggers a natural convection flow in the atmosphere surrounding the sensing element. Though such a flow can help transporting the substance to be detected by interacting with the outside air through the package holes, however it is necessary that the natural convection forces the air in the sensor to be expelled and allows new air to come in. This process of air exchange is strongly related to the shape and position of package apertures and to the orientation of the package.

The classic TO8 package used for gas sensors is a metal package made by a metal base with some pins and a cylindrical metal cap. The diameter and the height of TO8 are about 13mm. The cap on top has a hole of 7mm diameter and a grid to allow gas propagation in the package. The grid does not affect significantly the gas diffusion process but creates a relatively strong resistance to air flows compared with an open hole.

The reference sensor used in this work is a nanostructured material based sensor deposited on an alumina substrate. The alumina is about 6mm x 6mm x 300µm and has metal traces on both sides. On one side a platinum heater is

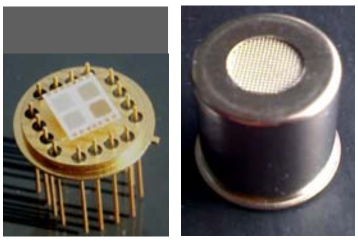

**Figure 1.** Standard TO8 package:
a) base with the suspended sensors array;
b) cap with hole and grid on top

placed, while on the other side a platinum thermometer is located along with four fingered contact areas where different metal oxides are deposited by a Pulsed Microplasma nanoparticles source [5] [6]. Metal oxides react in different ways with various gases, reducing or increasing their electrical conductance, which is measured and processed in order to ascertain whether some gases are present in the atmosphere and measure their concentrations [2] [3] [4]. This sensor works at about 600K and this temperature has been employed for investigation in this work. To avoid problems due to different thermal expansion of various materials and to simultaneously provide a suitable thermal insulation preventing excessive energy consumption in the heater, the alumina substrate is suspended in the package by bonding wires.

## 2. Simulation method

As explained earlier, this work aims at studying natural convection within the package with the goal to propose a new package with optimized apertures that improve the air exchange in all orientations. An optimization of the air exchange between the environment and the atmosphere inside the cap becomes necessary for being able to detect very small gas concentrations (parts per million or lower). As a matter of fact, if gas concentrations are very low sensors risk to detect nothing for a long period of time. Optimizing the air flow through package apertures should provide higher sensor's efficiency by helping the few gas molecules in the atmosphere to reach the sensor's surface and to be detected.

Multiphysics finite elements (FE) simulations are used to model the air flow within the package, and the main parameters considered to evaluate the performance of the package are the average air flow entering and exiting the package. Simulations are carried out in Comsol using the predefined equations of *Incompressible Navier-Stokes* and *Convection and Conduction*, with the coupling available in Comsol main module.

The main problem with FE simulations of natural convection is that it is difficult to get convergence. For convergence it is better to have a homogeneous meshing on the whole simulation domain. The mesh must be quite fine with mild density to adapt to the smaller structure and to avoid an excessively large number of variables. Some approximations are needed to reduce the geometry to a two-dimensional domain as a three dimensional model would be computationally too heavy for a common workstation. The two-dimensional approximation is achieved by simulating only a slice of the system and then extend results to the whole system using symmetry. Two positions of the package, with pins on bottom and with pins on top, have been analyzed. In the analyzed sensor, the alumina chip is suspended by the bonding wires to avoid problems due to heat sinking and thermal expansion of different materials. Bonding wires have been neglected in simulations because their size is very thin compared with sensor and package. The model includes the alumina, the package with a slice of the grid, and a volume of air located inside and outside the package. The heater power is simulated by a simple mathematical relation that expresses the power dissipated point by point within a thin portion of the alumina block. The temperature control is mathematically performed comparing the desired temperature with the average temperature recorded from alumina side.

Due to convergence issues, it is necessary to run transient simulations, evaluate it manually and obtain a stationary solution when the initial transient has been exhausted and the distribution of temperature and air velocity is constant. It is important in this respect to note that a stationary solution is to be expected, as the Rayleigh number $R_a$, i.e. the dimensionless parameter controlling thermal convection, attains relatively low values. More precisely, for an infinite layer of fluid of thickness $D$, characterized by thermal diffusivity $k$, kinematic viscosity $\nu$, coefficient of thermal expansion $\alpha$, the Rayleigh number $R_a$ reads:

$$R_a = g\, \alpha\, D^3 (T_1 - T_2) / k\, \nu\,, \qquad (1)$$

where T1 is the temperature of the lower hot boundary and T2 is the temperature of the upper cold boundary. Though the geometry of the present configuration differs from an infinite layer due to the presence of the confining cylinder, however, the use of the above definition leads to a simple estimate of $R_a$, which may provide some qualitative suggestion on the nature of thermal convection. In fact, the estimated values of $R_a$ range about few tens of thousands. It is then reasonable to expect that convection keeps laminar and convection cells are steady. On the other hand, one may estimate a Reynolds number

$$R_e \,(\equiv U\,D\,/\,\nu) \qquad (2)$$

with $U$ scale for the flow velocity. As discussed below, $U$ does not exceed few cm/s, hence $R_e$ ranges about few tens, an estimate which confirms the laminar picture.

The results also strongly depend on external air flows. However, such flows are neglected here, as they are unpredictable. If the sensor is placed inside a cabinet, as done most of the times, external air flows are not very strong and in that event the model presented here approximates the real situation very well.

## 3. Simulation Results

First set of simulations, modeling the classical TO8 sensor package without modifications, shows that the air flow is very low, when the package is vertical "face down" compared with the package "face up". In fact, if the hole in the package is on the bottom side only and the heater is in the upper part, the hot air stands still in the upper part of the package where the heater continues to heat it and hence no free convection is possible. In the simulation results, shown in Fig. 2 and Fig. 4, the color on the surface is proportional to the temperature point by point and a grid of arrows visualizes the velocity field in the air domain. It is then clear that, for the package with the grid on top, an air exchange is possible but strongly limited by the presence of the filter grid, while for the solution with the grid on bottom, the air starts to circulate

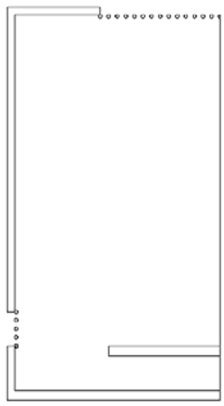

**Figure 3.** Proposed new package (half section, symmetry axis at right)

in a small part of the package, without a real exchange with the external environment. Values of air speed near the hole are about $4{\cdot}10^{-2}$m/s for the package with hole up, and $4{\cdot}10^{-5}$m/s for the package with hole at bottom.

## 4. Proposed Modification

Following the results presented earlier, a modified package – aimed at enhancing air circulation is proposed. This is obtained by inserting 1mm high windows on the vertical walls adjacent to the sensor (see Fig. 3).

Simulations with new package show that in "face up" configuration the air flow is almost the same as that in the old package, but with much less vortices. Moreover, most of the new air entering the package flows along the sensor

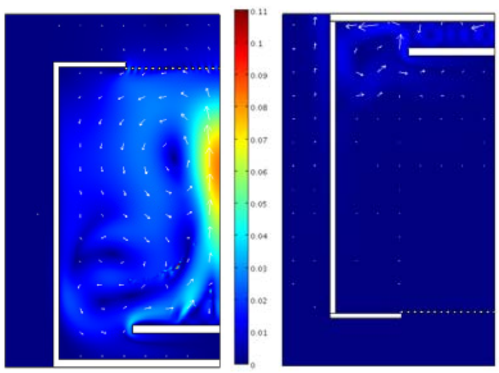

**Figure 2.** Standard package simulation results for face up and face down orientations: arrows and color scale indicate air speed direction and value (m/s)

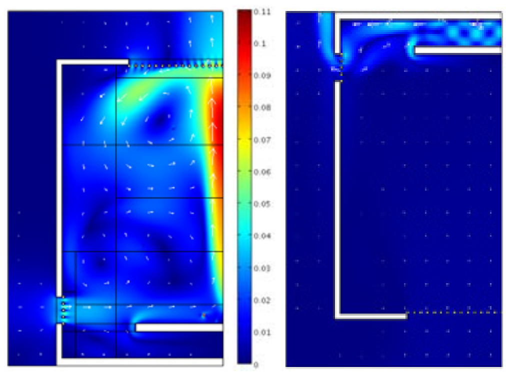

**Figure 4.** Proposed package simulation results for face up and face down orientations: Arrow and color scale indicate air speed direction and value (m/s)

**Table 1.** Results summary

| | Standard package face up | Standard package face down | Modified package face up | Modified package face down |
|---|---|---|---|---|
| Average inlet velocity [m/s] | $4{\cdot}10^{-2}$ | $4{\cdot}10^{-5}$ | $5{\cdot}10^{-2}$ | $5{\cdot}10^{-3}$ |
| Average outlet velocity [m/s] | $4{\cdot}10^{-2}$ | $4{\cdot}10^{-5}$ | $6{\cdot}10^{-2}$ | $2{\cdot}10^{-2}$ |
| Average exchange flow [$m^3$/s] | $6{\cdot}10^{-7}$ | $6{\cdot}10^{-10}$ | $1{\cdot}10^{-6}$ | $2{\cdot}10^{-7}$ |

surface and thus provides an optimal condition for the sensing process.

A major improvement is also achieved with the package in the “face down” orientation as, in that case, the windows are in the upper part - where hot air accumulates. The windows allow the air to flow out of the package, enabling new air from the circular hole on the bottom face to come in. This allows the flow to reach the same values as that of “face up” orientation, with an about 1000 times increment.

Table 1 summarizes the estimated air speed and the exchange flow for the two examined orientations. It can be noticed that the modified package improves the air exchange and consequently the efficiency of the sensor. Furthermore, the difference between air exchanges in different positions is reduced and the sensor, in the proposed new package, seems not to have a preferred orientation for best performance.

At this point some comments are to be made about the accuracy of the numerical predictions.

It would be important to show that the presented solutions are mesh independent. Some preliminary tests have been made by increasing the mesh size to be able to compare the velocity fields in different mesh cases. Some inconsistencies are found which show that the mesh with “larger” size is not yet appropriate as important details are missed. When trying to reduce the mesh size, convergence problems occur. The problem under analysis is computationally too heavy to be solved with a common workstation and it would require more powerful tools. This critical point is under analysis and some confirmations are expected in the next future.

## 5. Conclusions

A new package has been proposed and first results suggest that it is likely to improve the efficiency of the sensor. The proposed package may also help in applications that require a specific orientation of the sensor which is not optimal for sensing efficiency. For instance, in a common smoke detection system the sensing units are attached to the roof of the room and sensors need to be placed with the pin side on top.

Future developments will include simulations with the same package in a horizontal position.

## 6. References


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