# Simulation of CO Gas Sensing by Molybdenum Oxide using COMSOL Multiphysics

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## Abstract

This paper reports simulation of Carbon Monoxide (CO) gas sensing by Molybdenum Oxide (MO) sensor using COMSOL Multiphysics software. Adsorption reactions on MO sensor were defined in Reaction engineering and the sensor was modelled in space dependent node. CO was injected through Gaussian pulse feed inlet at 1 to 5 ppm into the gas chamber and MO sensor layer was allowed to reach steady state. Simulation results showed change in surface concentration of the adsorbed CO molecules on the sensor layer with change in CO concentration. Maximum surface coverage at CO concentrations of 1 ppm, 3 ppm and 5 ppm were 34.63 %, 55.08 % and 67.33 % respectively. The simulation results were in good agreement with that of the predicted by Langmuir Adsorption Model with a maximum error of 13 %.

***Keywords:*** *Adsorption, CO Gas, Molybdenum Oxide, COMSOL Multiphysics*

## 1.0 Introduction

Air pollution is caused due to the presence of harmful gases such as ammonia, carbon monoxide (CO), Sulphur dioxide and methane. Presence of CO is mainly due to IC engines emissions, industrial waste, sewage leaks, and mines [1]. CO gas sensors are required to monitor CO in the atmosphere. Metal Oxide Sensors (MOS) measure gas concentration by detecting change in resistance of metal oxide sensors as a result of gas adsorption. MOS have numerous advantageous such as high selectivity, high sensitivity, short response and recovery time. Some of the disadvantages include high operating temperature (100 to 450 $^0$C), degradation of sensor layer over long run, high power consumption (100 mW to 1 W) [1, 2]. Widely studied MOS gas sensing materials are N-type materials contributing 85 % of gas sensors market [2]. Some of the

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N type MOS gas sensor materials are Tin oxide, Indium oxide, MO and Titanium oxide. MO is one such MOS sensor material with superior chemical and physical characteristics making them versatile and tuneable for gas sensing [3]. Ciftyurek et al. [4] investigated molybdenum and tungsten binary and ternary oxide thick films on a chemiresistive sensor platform for monitoring of $SO_2$ gas. Evaluated $SO_2$ sensitivity of Molybdenum trioxide ($MoO_3$), Stronium molybdate ($SrMoO_4$), Nickel molybdate compositions at 600 to $1000^0$C. $SrMoO_4$ composition was found to be more sensitive, stable and selective to $SO_2$ gas up to $1000^0$C. Prasad et al. [5] reported gas sensing properties of Ion beam sputter deposited $MoO_3$ thin films. The authors measured change in DC conductivity in the presence of 490 ppm $NH_3$, $NO_2$, $C_3H_6$, CO and $H_2$. At $440^0$C, the film was found to be sensitive to $NH_3$ with 490 ppm increasing the conductivity by a factor of 70. This response was unaffected by 100 ppm concentration of accompanying gas.

Kumar et al. [6] showed a numerical model to explain the sensing principle of MOS gas sensors. A numerical model of chemical adsorption of $O_2$, CO and water vapour on the surface of $SnO_2$. Surface coverage of chemically adsorbed $O_2$ molecules was simulated as a function of $O_2$ pressure, temperature of sensor surface, and bulk doping level N type $SnO_2$ semiconductor material. Niyat and Abadi [7] performed simulation of MOS sensor which was a P-N hetero junction formed by $SnO_2$/ rGO. Exposure model, Heat transfer model and Electrical model simulations were performed using COMSOL Multiphysics. These results were found to be in good agreement with the experimental results. Arun et. al [8] performed simulation on ZnO based gas sensor for detecting acetone using COMSOL Multiphysics. A meander shaped micro heater was used to heat the sensor to optimum operating temperature of 423 K and variation of temperature with respect to input voltage was studied. Variation of response of sensors with change in concentration of acetone was simulated.

Review of open literature [1-8] indicated the potential of numerical solvers such as COMSOL Multiphysics for predicting the behaviour of gas sensors. The objective of this research was to perform simulation of gas sensing mechanism of MO sensor using COMSOL Multiphysics when exposed to different concentrations of CO gas.

## 2.0 Simulation

Simulation was performed using Reaction engineering, Transport of diluted species, Surface reactions and Laminar flow physics interfaces in COMSOL Multiphysics software. Two kinds of simulations, namely,

space independent and space dependent simulations were performed on MO in a constant volume gas chamber. Space dependent 3D simulation was performed using the results obtained from that of the space independent. Fig. 1 shows the procedure followed for the modelling and simulation of MO sensor for CO sensing.

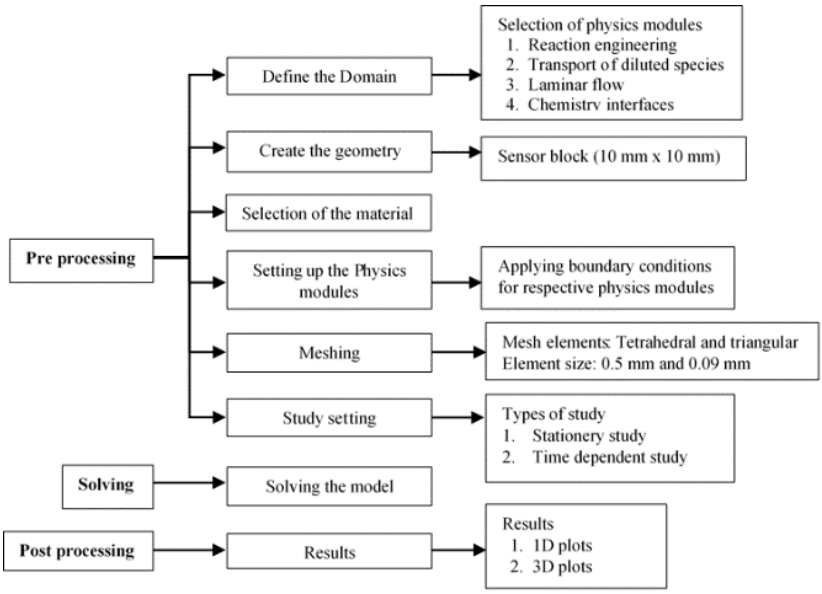


**Fig. 1.** Modelling and Simulation of gas sensing

Geometry of the sensor was modelled as a block of 10 x 10 x 0.2 $mm^3$. Tetrahedral elements were used as primary mesh to mesh the sensor body with element size of 0.5 mm. Triangular elements were used to create fine mesh on the sensor surface with an element size of 0.09 mm, as shown in the Fig. 2.

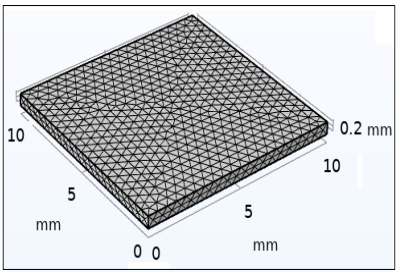


**Fig. 2.** Meshed sensor

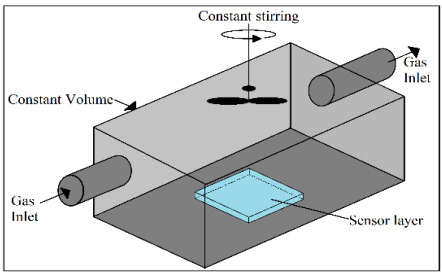


**Fig. 3.** Boundary conditions

Fig. 3 shows the boundary conditions used in the simulation. MO sensor layer was exposed to CO gas in a constant volume chamber with the injection of gas through gaussian concentration pulse feed inlet at a constant feed rate of $5x10^{-7}$ $m^3/s$. The target gas was injected at concentrations of 1, 3 and 5 ppm. Table 1 presents the parameters used in

the simulation to study the variation of surface coverage with respect to change in CO concentration.

**Table 1.** Parameters used in the simulation

| Parameter | | Unit | Description |
|---|---|---|---|
| $A_{surf}$ | $7.85x10^{-5}$ | $m^2$ | surface reaction area on sensor surface |
| $V_{fp}$ | $5.03x10^{-7}$ | $m^3/s$ | volumetric feed to the inlet |
| U | $1x10^{-4}$ | m/s | average fluid velocity within chamber |
| $G_0$ | $2.30x10^{-5}$ | $mol/m^2$ | initial site density of reactive surface |
| $M_{co}$ | $2.80x10^{-2}$ | kg/mol | molar mass CO gas |
| $M_{o2}$ | $1.60x10^{-2}$ | kg/mol | molar mass $O_2$ gas |
| $K_{co}$ | 15 | - | equilibrium constant for CO adsorption reaction |
| $K_{o2}$ | 31.318 | - | equilibrium constant for oxygen adsorption reaction |

## 3.0 Results and Discussion

Simulation results at CO gas concentrations of 1 to 5 ppm are presented in Fig. 4. CO was injected into the gas chamber containing MOS sensor layer and was allowed to attain steady state at each concentration.

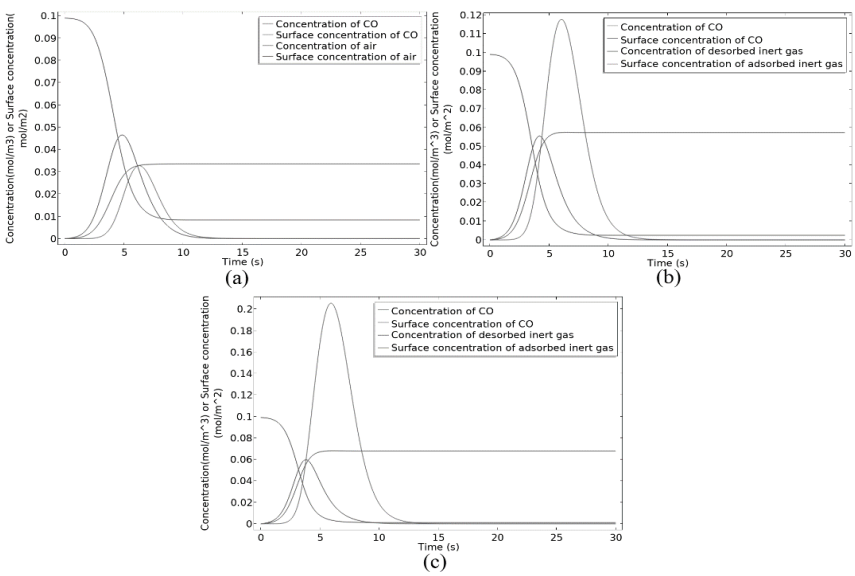


**Fig. 4.** Surface concentration vs time at a) 1 ppm, b) 3 ppm and c) 5 ppm of CO exposure

Initially, adsorbed inert gas present on the sensor layer led to high surface concentration of adsorbed inert gas at time t = 0 s. As time progressed (Fig. 4a) peak of the injection of target gas was observed at time t = 5 s. The injection is through gaussian concentration pulse feed inlet, which has a characteristic bell-shaped curve, showing that during injection, the

concentration gradually increased to a maximum and then dropped to the baseline in a specified time of 9 s.

As the adsorption proceeded, surface concentration of CO decreased. The reason for this raise and fall of surface concentration of the species is due to availability of finite number of active sites on the sensor layer. Since the number of sites are limited, it is essential for one species to get desorbed when a new species has to get adsorbed on these sites and the selectivity of which gas gets adsorbed and which gas gets desorbed depends on the relative affinity of these respective gases with the sensor layer. CO gas has greater affinity towards MO sensor layer than that of the inert gas because of residual attractive forces present on top of the sensor layer which attracts CO gas more strongly than the inert gas. After some time, most of the inert gas gets desorbed from the surface and is replaced with CO and $O_2$ gases. These gases start reacting on the sensor surface to form redox products and finally gets desorbed from the surface. Fig. 4b and Fig. 4c show the surface concentration of different species (CO, $O_2$) with respect to time at 3 ppm and 5 ppm inlet gas concentrations respectively.

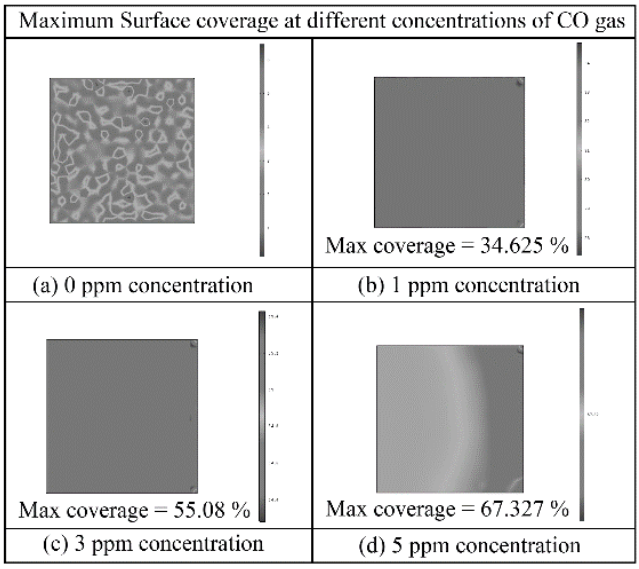


**Fig. 5. a-d). S**urface coverage at different concentrations of CO gas

Fig. 5a to 5d shows 3D plots for maximum surface coverage of CO on MO surface at different concentrations of target gas. At 0 ppm no adsorption of gas molecules on the surface, at 1 ppm the adsorption is more uniform due to availability of large area of active sites with coverage of 34.63 %. At 3ppm with coverage 55.08 % and 5 ppm with coverage 67.33 %. It can be observed that as the gas concentration

increases, the adsorption uniformity decreases due to limited availability of active sites on the surface. The plots clearly show that as the gas concentration in the test chamber increases, there is an increase in number of adsorbed molecules on the surface which results in increase in surface coverage. The surface coverage of the chemically adsorbed gas molecules behaves as a function of gas concentration, as predicted by Langmuir adsorption model.

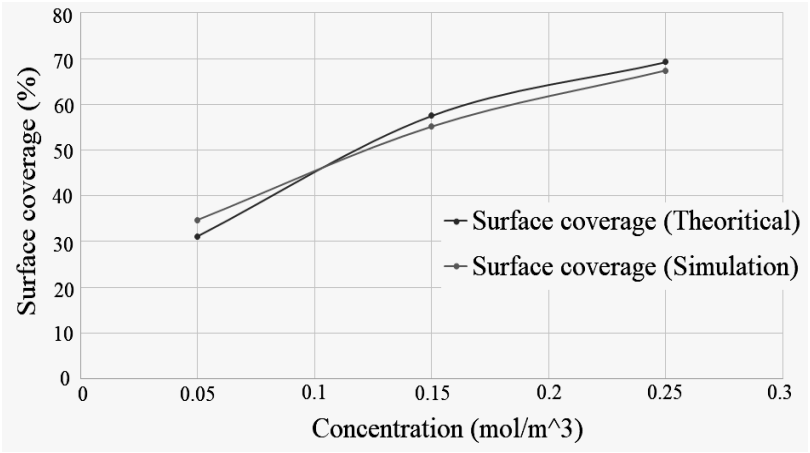


**Fig. 6.** Surface coverage vs concentration

Fig. 6 shows surface coverage vs. gas concentration. At the beginning of adsorption, the rate of increase in surface coverage is high. This is because of start of formation of monolayer adsorption on the sensor surface. As the concentration increases, there is very large number of molecules ready to adsorb near the surface. Hence a greater number of molecules strike the surface and lose their energy as heat to get adsorbed on the sensor surface (exothermic nature of adsorption). Once the sensor surface is completely covered with monolayer adsorbed gas molecules, multilayer adsorption formation starts given the gas concentration is still kept on increasing. This adsorbed gas molecules alter the conductivity of the MO sensor layer by hindering the free flow of electrons in conduction band. If these adsorbed gas molecules react with adsorbed oxygen ions on the sensor layer, they get reduced and gets desorbed from the surface as chemically stable product leaving behind the charge carriers in the sensor material, which results in conductivity change. In other words, change in surface coverage is indication of change in the conductivity of the sensor material, which is a useful property in gas sensing applications.

## 4.0 Conclusion

MO sensor was modelled and adsorption simulation was performed using COMSOL Multiphysics software. Molybdenum oxide sensor layer was exposed to CO gas in a constant volume chamber with injection of gas through gaussian concentration pulse feed inlet at a constant feed rate of $5x10^{-7}$ $m^3/s$. The target gas was injected at concentrations of 1 ppm, 3 ppm and 5 ppm. At the start of adsorption process, the rate of adsorption was observed to be high and it gradually reduced and attained steady state over the time. The adsorption profile showed edge effect during development. The maximum surface coverage at concentrations of 1 ppm, 3 ppm and 5 ppm were 34.63 %, 55.08 % and 67.33 % respectively.

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