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CONTROL-ORIENTED INVESTIGATION OF SWITCH-TYPE AIR/FUEL RATIO SENSORS

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Abstract: During the next years, the limiting values for NO_X, HC, and CO concentrations in the exhaust gas of an SI engine will be further lowered by legislation. This makes improvements of the existing pollution control systems indispensable. In order to apply an effective control system, the dynamics of the Three Way Catalytic Converter (TWC) have to be analysed properly. Therefore, much attention has been paid to the modelling of the TWC in various investigations during recent years. However, less attention has been paid to the oxygen sensors and their behaviour upstream and downstream the TWC, especially during transients.

This investigation focuses on the behaviour of the switch type air/fuel ratio sensor upstream and downstream the TWC both in steady-state and transient operating conditions. For this purpose a detailed model of the sensor has been derived, which fits the measurement data very well. The model has been inverted in order to calculate sets of gas concentrations which lead to a specific sensor voltage output. This allows a better interpretation of the measured air/fuel ratio transients in terms of TWC observation and thus an improvement of control oriented modelling of the TWC.

Keywords: Lambda Sensor, Three Way Catalyst

1. INTRODUCTION

The lowering of the the limiting values for NO_X, CO and HC in the past and in the future makes the exploitation of the TWC's storage capacity imperative. Therefore, an appropriate observer of the TWC with its oxygen storage capacity has to be incorporated in the control system. During the recent years, many attempts have been made in the field of TWC modelling. Thereby, mostly the focus was on the estimation of the oxygen storage level and/or the air/fuel ratio downstream the TWC. Meeting the limititations of the mentioned species is about to be successfully implemented in state-of-the-art control systems. However, a further improvement can make a significant reduction of the TWC's noble metal loading possible.

A closed-loop observer for the estimation of the TWC's storage level can only be applied, if an appropriate sensor information can be obtained to support and — if necessary — correct the observer. For this purpose, usually the second lambda sensor downstream of the TWC is used, see e. g. (Gerhart *et al.*, 1998). Yet two main problems arise with this configuration. Firstly, it has been shown in various investigations that lambda sensors exhibit cross sensitivities towards species such as hydrogen. During transient operation, excursions of the hydrogen concentration can significantly disturb the sensor signal. Secondly, it is not entirely clear, how the lambda sensor's output corresponds to the oxygen storage level in the TWC.

In order to obtain a deeper insight into the lambda measurement and in order to be able to better interpret the sensor's outputs, a detailed model of a switch-type lambda sensor has been derived. The details of the model have been presented previously, (Auckenthaler *et al.*, 2002).

2. MODEL OF A SWITCH-TYPE LAMBDA SENSOR

The sensor model consists of three modules:

(1) Thimble and the porous protection layer
(2) Catalytic electrodes
(3) Electrolyte

Only the first and the second modules are modelled dynamically, the third module is static.

The first module describes the diffusion through the thimble and the porous protection layer onto the catalytic electrodes. It calculates the partial pressures of the species at the electrode surface from the partial pressures in the exhaust gas and from the production terms arising from adsorption and desorption on the electrode. This part has been modelled by the use of Stefan-Maxwell equations:

$$J_i = \frac{-\frac{p}{\Re T} \cdot \nabla p_i + p_i \cdot \sum\limits_{j=1, j\neq i}^{n} \frac{J_j}{D_{ij}}}{\sum\limits_{j=1, j\neq i}^{n} \frac{p_j}{D_{ij}}} \tag{1}$$

J_i denotes the mass flux of the species i in $\mathrm{mol\,m^{-2}s^{-1}}$. p, $\Re$ and T stand for the total pressure, the universal gas constant and the temperature. p_i is the partial pressure of the species i and D_{ij} the binary diffusion coefficient of the species i diffusing into j.

The catalytic electrodes are modelled in the second module. Thereby, the occupancies of adsorbed species and reaction products are calculated from the partial pressures of O_2, H_2, CO, H_2O, and NO. HC have been neglected, since they only exhibit little influence on the sensor model's voltage output, (Auckenthaler *et al.*, 2002). The occupancies of the following species have been taken into account: O, H, OH, H_2O, CO, C, NO and N. In addition to the occupancies, also the production terms from adsorption and desorption are calculated in this module. Apart from the adsorption and desorption of the mentioned gas species, the following reactions have been considered:

$$\begin{aligned}
\mathrm{CO + CO} &\rightarrow \mathrm{C + CO}_{2,g} \\
\mathrm{C + O} &\rightarrow \mathrm{CO} \\
\mathrm{CO + O} &\rightarrow \mathrm{CO}_{2,g} \\
\mathrm{O + H} &\rightarrow \mathrm{OH} \\
\mathrm{OH} &\rightarrow \mathrm{O + H} \\
\mathrm{OH + H} &\rightarrow \mathrm{H_2O} \\
\mathrm{H_2O} &\rightarrow \mathrm{OH + H} \\
\mathrm{OH + OH} &\rightarrow \mathrm{H_2O + O} \\
\mathrm{NO} &\rightarrow \mathrm{N + O} \\
\mathrm{NO + N} &\rightarrow \mathrm{N}_{2,g} + \mathrm{O} \\
\mathrm{N + N} &\rightarrow \mathrm{N}_{2,g}
\end{aligned} \tag{2}$$

In the third module, the sensor's Voltage output E is calculated from the occupancy of O, H, OH, CO and C. All the electrochemical reactions and ion transitions between the electrodes and the electrolyte have been lumped into the following static equation:

$$E = \frac{\Re T}{2F} \cdot \left[\log\left(\frac{\vartheta^4_{O,\mathrm{ref}}}{\vartheta^4_O + \frac{k_{a,OH}}{k_a}\vartheta^2_{OH} + \epsilon} \right) + \log\left(1 + \frac{k_{f,C}}{k_f}\vartheta^2_C + \frac{k_{f,CO}}{k_f}\vartheta^2_{CO} + \frac{k_{f,H}}{k_f}\vartheta^2_H \right) \right] \tag{3}$$

ϑ_i denotes the occupancy of the species i. F is the Faraday constant. ϵ stands for a saturation term which can be interpreted as the minimal oxygen ion concentration in the boundary layer of the electrolyte, if no reducing species are present.

The sensor model has been tested at various operating points upstream and downstream of the TWC. The concentrations of O_2, H_2, CO, CO_2, NO, and HC together with the corresponding output voltage of the lambda sensor have been measured on a modern production type V6 SI engine. The concentrations of H_2O and N_2 have been calculated from mole- and mass balances. The concentrations of one operating point are shown in figure 1 as functions of the air/fuel ratio, λ.

The static response of the model at 930 K is shown in figure 2, when applied upstream of the TWC and in figure 3, when applied downstream. The correspondence with the measurements is very good. Notice the second augmentation of the voltage at λ=0.95, which is very well reproduced by the model. The slight offset of the sensor's characteristic to the lean side is caused by the offset of the wide-range lambda sensor. The outputs of the latter have been used for the x-axis. Since the same λ-values have been taken for the gas composition measurements (figure 1), simulation and measurement are consistent.

The model allows to analyze the sensitivities towards different exhaust gas components. It has been shown in (Auckenthaler *et al.*, 2002) that the sensitivity towards hydrogen is significant. The reason for this is the fact that the voltage is only

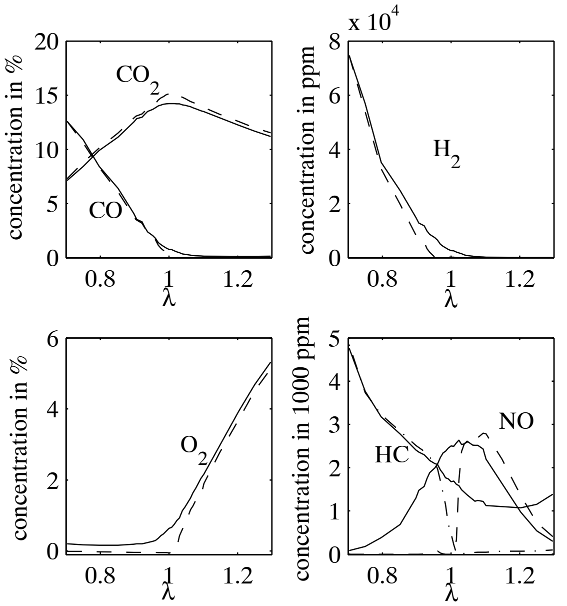

Fig. 1. Measured exhaust gas composition for the sensor model in one operating point. Solid lines represent concentrations upstream of the TWC, dashed line downstream of the TWC.

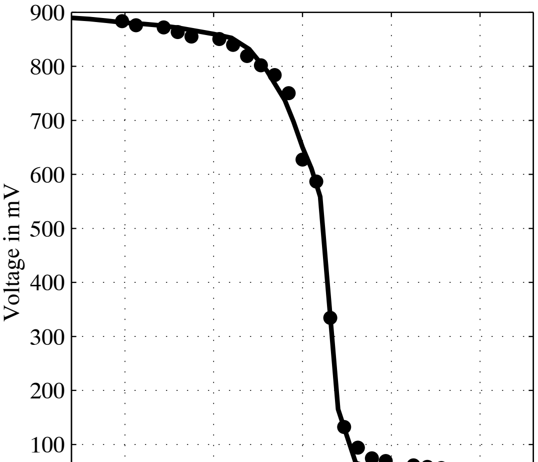

Fig. 2. Simulated characteristic of a switch-type lambda sensor upstream of the TWC at 930 K. Measurements are represented by bullets. λ-values are measured with a wide range sensor.

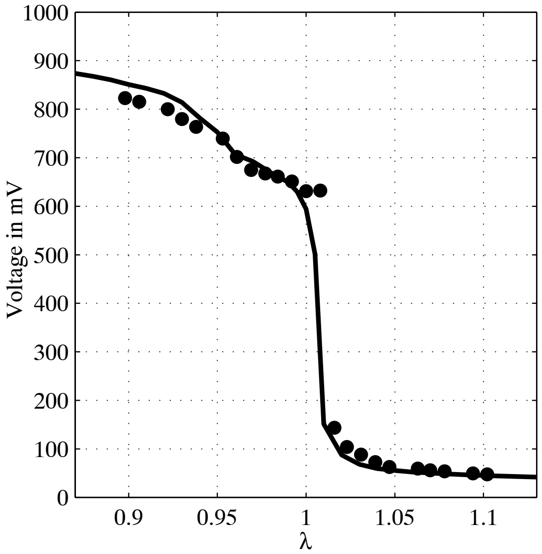

Fig. 3. Simulated characteristic of a switch-type lambda sensor downstream of the TWC at 930 K. Measurements are represented by dots. λ-values are measured with a wide range sensor.

partly driven by the shortage of oxygen in the exhaust gas. This is in contrast to the widely used Nernst equation when applied to the oxygen concentrations. In (Bozek *et al.*, 1992), it was shown that the voltage of a switch type lambda sensor can only reach 400 mV, when exposed to a pure inert gas such as nitrogen. In the same investigation it was shown that the sensor reaches about 600 mV when exposed to carbon monoxide diluted in an inert gas and above 800 mV when exposed to diluted hydrogen.

Physically, the voltage does not arise from the oxygen concentrations in the gas phase, but rather from the oxygen ion concentrations in the outer layers of the electrolyte. This concentration is only partly driven by the oxygen concentration in gas phase. It is also driven by the reducing species which are adsorbed on the electrode or on the electrolyte. The electrical potential, i.e. the voltage, equals the chemical potentials of the redox- and the oxygen transfer reactions at the three-phase boundary gas/electrode/electrolyte. Therefore, the sensor exhibits significant "cross sensitivities" towards reducing species.

3. INVERSION OF THE MODEL

As has been mentioned in the previous section, the sensor exhibits cross sensitive behaviour towards hydrogen. During transients, a TWC can release significant amounts of hydrogen in any operating condition, i. e. with a rather full or empty oxygen storage level. Observer based controllers of the TWC usually translate the downstream lambda sensor signal into the oxygen storage level. Hence, the hydrogen excursions can lead to a wrong interpretation of the sensor signal and thus to significant disturbances of the oxygen level controller.

Oxygen level controllers try to keep the level and thus the lambda sensor output constant. In this section, the inversion of the presented model will be derived. This inversion allows to calculate all

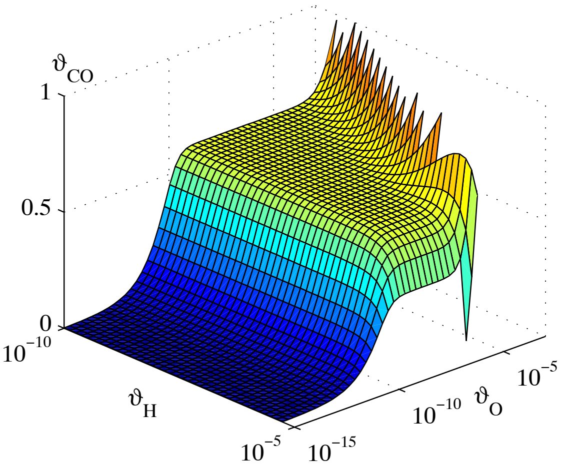

Fig. 4. Occupancy of CO at low NO (0.01) and H_2O (10^{-6}) coverages at 600 mV and 930 K.

possible exhaust gas compositions which may lead to a specific lambda sensor output.

The lambda sensor dynamics are much faster than the TWC dynamics. Therefore, the inversion is derived from the static model, i. e. all derivatives in time are assumed to be zero. At first, the third module has to be inverted, which is described by equation 3. The goal is, to calculate the occupancies of C, CO, OH and N from the occupancies of O, H, H_2O and NO at a specific Voltage. In a second step, the partial pressures of the gas components adjacent to the electrode, and the production terms, which arise from adsorption and desorption, are calculated. This can be seen as the inversion of the second module. Finally the first module will be inverted, which gives the partial pressures of the different gas species.

The mathematical details of the model inversion shall not be presented here, since a considerable amount of elementary algebraic operations is involved. The inversion is straight forward and can be easily derived from the model information provided here and in (Auckenthaler *et al.*, 2002).

3.1 Occupancies

The voltage output is strongly dependent on the occupancy of O, H and CO. NO and H_2O are expected to show less influence. Therefore, the occupancy of CO as a function O and H at different NO- and H_2O-levels has been calculated. The occupancy of C, OH and N are obtained implicitly from the model. In figure 4, an example at low NO- and H_2O occupancies is presented. The Voltage is 600 mV and the sensor temperature 930 K. Additionally, the occupancy of C is presented in figure 5.

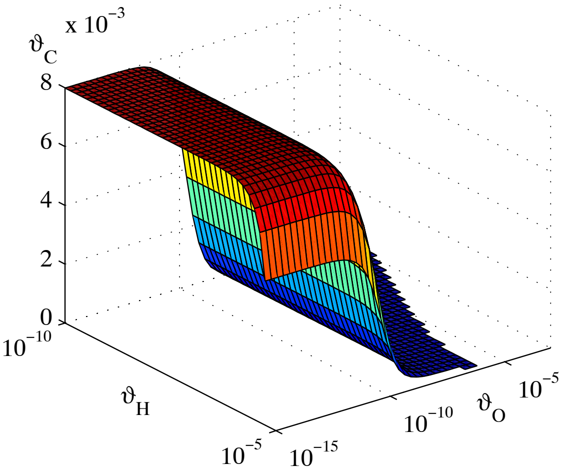

Fig. 5. Occupancy of C at low NO (0.01) and H_2O (10^{-6}) coverages at 600 mV and 930 K.

The variation of the CO occupancy in the area of low O occupancy occurs not because of the dependency on O, but rather because of the occupancy of C. The C concentration is higher at low O coverage and decreases with increasing O. Only at higher O occupancy, the CO coverage shows a dependency of O. The CO occupancy decreases fast with increasing H occupancy at H levels above 10^{-6}. This strong variation occurs because of the sensor's sensitivity towards hydrogen.

The occupancies presented here are only partially achievable in reality. Especially, when the conditions in an exhaust pipe of an SI engine are considered, where the total gas pressure is limited to approximately 1 bar. This is a very narrow limit as compared to the presented occupancies, which will be shown in the following sections.

3.2 Gas pressures adjacent to the electrode

The calculation of the partial gas pressures adjacent to the electrode have been performed under the condition of maximum total pressure of 1 bar. This condition narrows the band of achievable occupancies of H and O significantly. The partial pressures have been calculated from the kinetic equations derived from the chemical reaction scheme, (2) and from the adsorption/desorption terms. Figures 6, 7 and 8 show the partial pressures of CO, H_2 and O_2 as functions of ϑ_O and ϑ_H. The pressures of hydrogen and oxygen augment with the corresponding occupancies ϑ_H and ϑ_O, as is expected. The pressures of carbon monoxide and hydrogen increase with the rising oxygen occupancy, to make up for the higher availability of oxygen, which by itself would reduce the voltage. Increasing hydrogen occupancy reduces the partial pressure of carbon monoxide, since both species support the voltage.

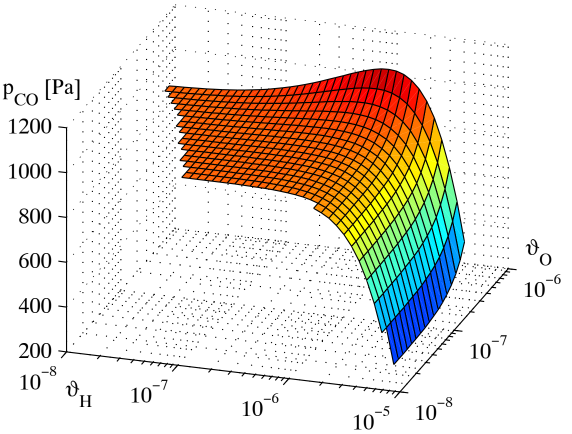

Fig. 6. Partial pressure of CO at the electrode at high NO and H_2O coverages at 600 mV and 930 K as a function of ϑ_H and ϑ_O.

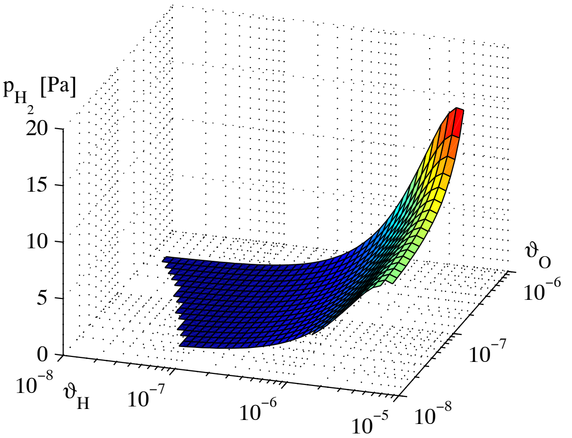

Fig. 7. Partial pressure of H_2 at the electrode at high NO and H_2O coverages at 600 mV and 930 K as a function of ϑ_H and ϑ_O.

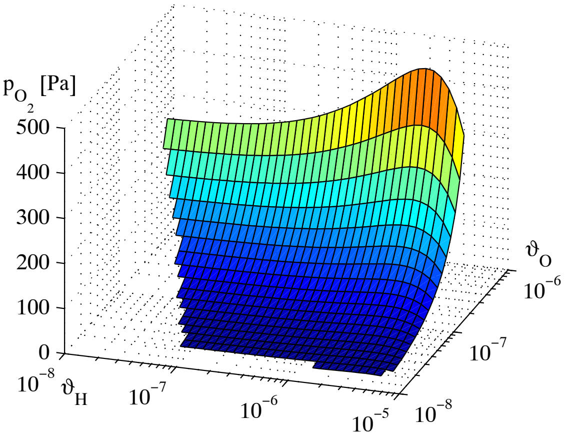

Fig. 8. Partial pressure of O_2 at the electrode at high NO and H_2O coverages at 600 mV and 930 K as a function of ϑ_H and ϑ_O.

3.3 Gas pressures at the thimble

As a final step, the pressures at the thimble of the sensor are calculated. These are the actual pressures in the exhaust gas. They have been derived from the Stefan-Maxwell equations (1). The mass fluxes of the various species are constant through the sensor at steady state conditions. They have been derived from the production terms arising from the adsorption and desorption on the catalytic electrode. Figures 9–13 show the partial pressures of CO, O_2, H_2, H_2O and NO as functions of ϑ_O and ϑ_H. The partial pressures of CO_2, N_2 and HC at the electrode have been fixed. These species do not have any influence on the inversion of the second module. However, they influence the diffusion. Therefore, they have to be accounted for in this part. The influence of their variations is assumed to be negligible.

The partial pressures of some species exhibit a considerable variation between the electrode surface and the thimble of the sensor. This shows the important influence of the hindered diffusion. It contributes to a great extent to the sensor's switch-type characteristic, since the shortages of reducing species on the lean side and of oxygen on the rich side are significantly amplified.

From figures 9–11 can be seen that even rather high oxygen partial pressures may be compensated by strongly increased CO and surprisingly weekly increased hydrogen partial pressures. This indicates that the sensor output might exhibit a high voltage, even if a considerable amount of oxygen is present. The oxygen concentration downstream of a TWC is an indicator for the oxygen storage level. Excursions of the hydrogen concentration may thus lead to a misinterpretation of the TWC's state, which can lead to breakthroughs of NO. Hence, if a switch-type sensor is applied downstream of a TWC, the concentrations of hydrogen and carbon monoxide have to be accounted for.

So far, these results are derived from simulation only, and have not yet been confirmed by measurements. However, the authors believe that the very good correspondence of the simulated sensor's characteristic with measurements in various operating points upstream and downstream the TWC strongly implies the correctness of the obtained results.

4. CONCLUSION

A model of a switch-type lambda sensor, which has been presented in an earlier investigation (Auckenthaler *et al.*, 2002), has been inverted. This inversion allows to calculate the ranges of partial pressures of O_2, CO, H_2, H_2O and NO, which lead to a specific voltage output of the sensor. It has been shown that high sensor output voltages can occur even at rather high oxygen concentrations, if the hydrogen and/or carbon monoxide levels are significant enough. Thus, the

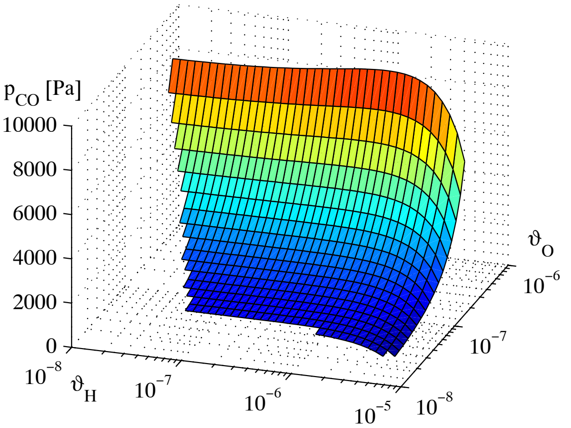

Fig. 9. Partial pressure of CO at the sensor at 600 mV and 930 K as a function of ϑ_H and ϑ_O.

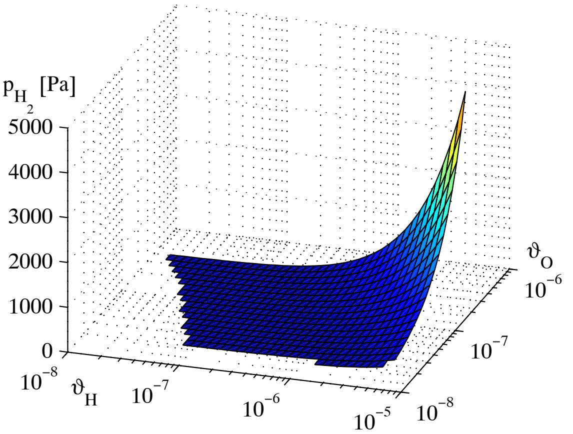

Fig. 10. Partial pressure of H_2 at the sensor at 600 mV and 930 K as a function of ϑ_H and ϑ_O.

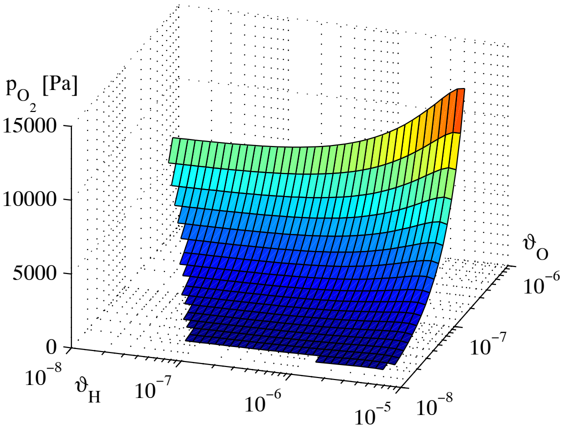

Fig. 11. Partial pressure of O_2 at the sensor at 600 mV and 930 K as a function of ϑ_H and ϑ_O.

partial pressures of the reducing species have to be accounted for when applying a switch-type lambda sensor downstream of a TWC to support an observer of the oxygen storage level.

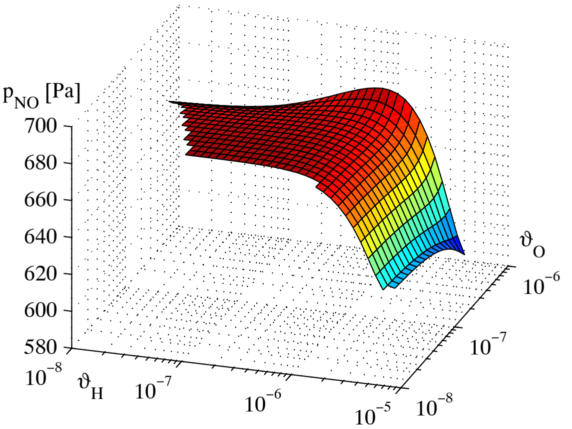

Fig. 12. Partial pressure of NO at the sensor at 600 mV and 930 K as a function of ϑ_H and ϑ_O.

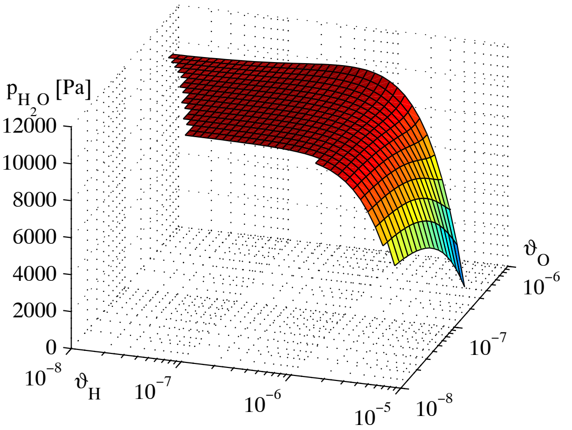

Fig. 13. Partial pressure of H_2O at the sensor at 600 mV and 930 K as a function of ϑ_H and ϑ_O.

5. ACKNOWLEDGEMENTS

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