

Artificial Olfactory Brain for Mixture Identification

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Experimental setup:

An array of 16 commercially available metal-oxide based gas sensors were placed in a 60ml volume test chamber. This chamber was connected to a computer-controlled continuous flow system that allowed us to obtain, starting from calibrated gas bottles, the desired concentrations of the different gases and gas mixtures in a highly reproducible way. The carrier gas was dry air. The total gas flow was set to 200 ml/min. Moisture level was kept at 10% R.H. (measured at $30^{\circ}C \pm 1^{\circ}C$). Both total gas flow and moisture level were kept constant during the entire measurement process. The following (four from each) screen-printed sensors by Figaro Inc. were used: TGS2620, TGS2610, TGS2602, TGS2600. A constant signal of 5V was injected to the polysilicon heating resistor of each gas sensor to reach the working temperature of the sensors equal to $400^{\circ}C$. This was done to measure the steady-state sensor response. A written-in-house LABVIEW program running on a PC platform was used for controlling the data acquisition board. The mission of this board was to acquire the dynamic response of gas sensors. To ensure that reproducible response patterns were acquired during each measurement the sensors were pre-heated for several days prior the experiment process get started.

The measurement procedure consisted of the following steps: First, a constant flow of dry air was circulating through the sensing chamber while the gas sensor array was kept at a stable working temperature of $400^{\circ}C$. In the second step, after 20s. the data recording started, the desired concentration of the gas was injected by the continuous flow system into the sensing chamber. Finally, in the third step (cleaning phase) the vapor was exhausted from the sensor array and the chamber was cleaned with dry air before the concentration phase of a new measurement could restart. The acquisition of these measurements took about 20 minutes to complete, i.e., 10 minutes for gas injection phase and 10 minutes for recovery (cleaning) phase. The recorded session in each measurement cycle was the first 100

seconds of the gas injection phase, where the resistances of all 16 sensors were acquired in parallel with sampling frequency of 100Hz. The manifold and measurements protocol (i.e., interval analyte dosing) had to be carefully designed, so that the dynamics of the transient sensor signal reflect the sensor-specific analyte diffusion and reaction characteristics rather than the gas flow dynamics of the setup and the measurement chamber.

Database:

We re-sampled the one-second long 100Hz records down to 1Hz by averaging every consecutive 100 samples, removed the offset from each sensor record, and re-scaled the odor period to 1s. This was done by mapping the odor period, which has fixed length of 100s in the original records, to 1s by re-indexing the time series.

The tables below lists the odors and their partial concentrations (in ppm) sampled in the measurements. Given a measurement among these records, the goal is to identify whether the applied odor is a pure toluene, a pure acetaldehyde, or any mixture of them. Note that the measurements are grouped into two datasets, each containing 40 measurements from highly imbalanced mixtures to be separated from pure odors.

The records in both datasets are provided in this supplementary material. Each record is given as an ASCII list of tab-separated 17 columns, where the first one is the re-scaled time index and the remaining 16 are the corresponding sensor resistances (after offset removal).

Table 1: Dataset 1 content

Odor		Vapor concentration				
Acetaldehyde	100	98	96	4	2	0
Toluene	0	2	4	96	98	100
Replicate	10	5	5	5	5	10

■ Pure Acetaldehyde

■ Mixture

■ Pure Toluene

Table 2: Dataset 2 content

Odor		Vapor concentration				
Acetaldehyde	50	49	48	2	1	0
Toluene	0	1	2	48	49	50
Replicate	10	5	5	5	5	10

■ Pure Acetaldehyde

■ Mixture

■ Pure Toluene

The Sample Antennal Lobe Model:

Throughout the simulations of this work, one particular topology generated by the Bernoulli process has been used.

The randomly generated connectivity of this topology (in the form of 150×150 adjacency matrix \mathbf{A}), the gains K_i^E, K_j^I , and time scales β_i^E, β_j^I $i, j = 1, \dots, 75$ are listed in the attached file `topology.net`. The first 150 lines of this ASCII file lists the rows of the binary matrix \mathbf{A} . The following line lists 150 values, the first 75 being K_i^E and the rest K_j^I . And the following (last) line lists β_i^E and β_j^I in the same manner.

The transpose of 16×150 sensor-to-AL connectivity matrix used in simulations is also provided in the file `sensormap.net`.

All other parameters of the model have been fixed to the values explained in Section 2.2. The scalar conductances g_E and g_I are determined as a separate procedure (as explained in the text) and they multiply the 75×75 lower-left and the 75×75 upper-right sub-matrices of \mathbf{A} , respectively, to determine w_{ij}^{IE} and w_{ij}^{EI} parameters the model. Note that the diagonal sub-matrices are zero since the model has no E -to- E nor I -to- I connections by construction.