

How Information-Rich are Sensor Response Interactions? Overlap and Resolution in Chemical Sensor Array Design

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Abstract:

Chemical sensor development often progresses by combining an analyte-dependent chemical phenomenon that induces a physical change with a transduction phenomenon responsive to that change. The effectiveness of the resultant sensor relative to other sensors is then considered in terms of a change in signal-to-noise or in “selectivity” as a result of the interplay between the underlying phenomena. Unfortunately, when arrays of these and/or related sensors are constructed, the aggregate capability of the resultant array underperforms expectations suggesting a significant overlap in the informatic capacity of the constituent sensors. This abstract presents a nascent theoretical approach and methodology for probing the overlap in sensing capabilities among sensors using mutual information and simple models for chemical sensing systems.

Key words Sensor Arrays, Quality Metrics, Mutual Information, Lock and Key Theory, Information Theory

Introduction

While there are many unknowns and technical challenges in chemical sensor array design, questions concerning the capabilities and limits of the underlying classes of sensors often go unacknowledged. For instance, the chemical activity of many cheap, light-weight, and fieldable chemical sensors such as metal oxide (MOX,) surface acoustic wave (SAW,) and microelectromechanical system (MEMS) type sensors are governed by surface adsorption-absorption/desorption (AA/D) phenomena of various analytes upon a thin film coated substrate [1].

In many cases, the same or similar thin films are used across multiple types of sensors with only the underlying transduction phenomenon to differentiate them. While this diversity problem is often empirically clear to the experimenter, the general impact of this problem from a theoretical and design standpoint is, in our view, unappreciated and under explored. The saliency of this problem only becomes more apparent when arrays of sensors are made [2] and, as is often the case,

increases in sensing capability are not found. Among sensors of the same type, there appear to be limited avenues for diversity from sensor to sensor.

Our guiding questions for this work are: How do we quantitatively assess the informatic differences between sensors of the same sensing mechanism? How do we compare sensors of differing sensing mechanisms? What are the capabilities and limitations of arrays constructed from permutations of these devices? What are the practical implications of such an analysis? Using a simple toy model, can we capture the essential AA/D properties of thin film coated sensors and reach insightful, practical conclusions?

Metrics and Models for Chemical Detection

We reframe these question in terms of an information capacity measure first explored by Huntley et. al. [3] for theoretically probing the lock-and-key binding model frequently employed in biological and soft matter investigations and a modified form of a toy model first used by Zwicker et. al. [4] for describing the sensing capabilities of biological

olfactory systems. By combining these approaches, we are able to explore the information richness or capacity of systems constructed from permutations of various AA/D chemical sensors.

We begin by defining a standard bound/unbound sensor model as given in [4]

$$s_n = \sum_i a_{ni} c_i \quad (1)$$

where s_n is the sum of the linear responses of sensor n to the analytes, c_i is the analyte concentration of analyte i and a_{ni} the strength of interaction between of interaction between the sensor n and analyte i . For theoretical convenience, we threshold this response

$$q_n = \begin{cases} 0 & s_n < t_n \\ 1 & s_n \geq t_n \end{cases} \quad (2)$$

where t_n is the threshold of sensor n . This model is intended to capture the essential features of an AA/D-based sensor in an active environment such as that depicted in fig. 1.

Next, we may measure the shared information between sensors or sensing systems using mutual information, defined as follows

$$I(X;Y) = \sum_{x_i \in X, y_i \in Y} p(x_i, y_i) \log_2 \frac{p(x_i, y_i)}{p(x_i)p(y_i)} \quad (3)$$

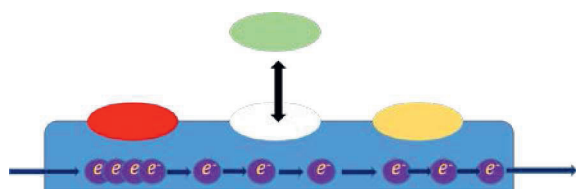


Fig. 1. A toy model of the influence of chemical adsorption and desorption upon electron flow in a sensing substrate.

where X and Y are two systems, x_i and y_i , their constituent component sensor responses and $p(\cdot)$ the relevant probability distributions.

Exploring the Limits of Sensing Phenomena

Using SAW sensors as a stand-in for the AA/D class of chemical detection, we are able to model the analyte sensitivity via a 5 parameter model of linear solvation energy as described in [7] The LSER parameter coefficients were estimated for each compound using Absolv from ACD/Labs. Partition coefficients for each

compound were estimated for 21 different polymer sensor coatings as described in [8].

Using equations (1)-(3) as well as the Ising model-type analysis described in [3]-[6], we are able to derive an estimate of the information capacity of the available polymers for the AA/D-based sensors. The effectiveness of these AA/D sensors for the detection of the trace analytes in [8] is then considered.

Acknowledgement

This work was funded by the Office of Naval Research/US Naval Research Laboratory. Dr. Knapp's postdoctoral fellowship was managed by and provided through the National Research Council's (USA) Research Associate Program.

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