Accelerating Analyte Quantification through Dynamic Sensor Calibration

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Chemical sensors have extensive applications in a variety of fields including environmental monitoring, human health diagnosis, and industry quality assurance. In many applications such as combustion control, sensors are often integrated with feedback controllers to fine-tune the operating conditions ([1], [2]). In those cases, the target analyte concentration is likely to vary rapidly, and real-time monitoring of the analyte requires a sensor which is able to keep up with the pace of the concentration changes.

Conventional sensor calibration seeks to associate steady-state sensor responses with the analyte concentration of interest through mathematical models. To achieve real-time monitoring within the scope of steady-state calibration, a sensor is required to be able to reach its steady state quickly (i.e., be highly responsive). Unfortunately, the commonly used electrochemical sensors and semiconductor-based resistive sensors usually fall short in terms of tracking the rapid changes of analyte concentrations, because of material limitations and underlying sensing mechanisms. Typically, it takes quite some time for a chemical sensor to reach its steady-state responses, that is, to complete multiple steps in the sensing signal generation: diffusion of the analyte to the sensor surface, adsorption of the analyte on the sensor surface, chemical interaction of the analyte with the sensor, and signal transduction. Consequently, there is a time lag between a sensor's steady-state signals and the environment changes. Through selection of sensing materials and/or sensor structure optimization alone, it is almost impossible to improve a sensor's response time performance to the extent that is acceptable to real-time monitoring [3]. In light of this, an appealing alternative is provided by dynamic calibration: modeling of a sensor's dynamic behavior so that its transient signals (as opposed to steady-state responses) can be used to track the analyte concentration.

To enable a sluggish sensor to real-time monitor the rapid changes in the analyte concentration, this work has developed a statistical method to calibrate the dynamic behavior of sensors. The dynamic calibration model takes the form of a polynomial transfer function (TF), and approximates the time-dependent relationship between $r(t)$, the sensor response, and $c(t)$, the possibly time-varying analyte concentration. The calibration models (i.e., the TF models) of a sensor have to be estimated from experimental data. To achieve a high-quality TF model, in this work, a design of experiments strategy was used for data collection, and an iterative model selection method was adopted to obtain the best TF model adequate to describe the sensor dynamics.

In this work, the dynamic calibration method has been applied to calibrate an electrochemical carbon monoxide (CO) sensor. It has shown that when coupled with the dynamic calibration model, the sensor is able to provide good estimates of CO concentrations within several seconds, whereas the time for the sensor to reach steady state is in the order of minutes. The proposed method is not limited to electrochemical sensors, which are used in this work for demonstration, but also can be applied to calibrate any sensor that exhibits exponentially decayed signals. As pointed out by Samitier et al. [4], many chemical sensors fall into this category.

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