Fluctuation dynamics in adsorption-based nanobiosensors

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When speaking of a biosensor we refer to a self-contained integrated device capable of providing specific quantitative or semi-quantitative analytical information using a biological recognition element which is in direct spatial contact with a transduction element (IUPAC definition, 1996). In a modern sense it is a sensor that integrates a biological element with a physicochemical transducer to produce an output signal (e.g. electronic or optical) proportional to the amount of a single analyte. This signal is then conveyed to a processing block which is often capable of conditioning and sending data to cloud, is equipped with smart displays, etc.). The specific biochemical reaction that we focus on here is physisorption, a reversible stochastic process of binding and un-binding between molecules at the sensing surface of the adsorbent and free moving adsorbate particles in a surrounding liquid or gas. Most often, the read-out mechanism of such affinity devices based on reversible adsorption, that we address is electromagnetic (through surface plasmon resonance, SPR), electrical (e.g. piezoelectric), electrochemical, etc. Nanobiosensors are nanostructured devices capable of detecting extremely low analyte concentrations (down to a single molecule).

In a mathematical sense, scaling down to nanoscale dimensions and to extremely low concentrations makes a great difference. The calculation apparatus valid for moderate analyte concentrations is usually based on the Lagergren model of adsorption. It allows for an easy estimate of all figures of merit in time and frequency domain (sensor response, sensitivity, linearity, selectivity), no matter whether we use a deterministic or a stochastic approach in our analysis. Models valid for extremely low concentrations are generally analytically unsolvable and must resort to extensive numerical computations instead. Fluctuation dynamics is essential both for determining the sensor response also for finding out the limiting performances due to stochastic fluctuations caused by adsorption (adsorption-desorption noise).

We present here the stochastic analysis of adsorption-desorption processes in different cases (mono-component and multicomponent adsorption, with and without steric effects). It is performed in different ways (by deriving expressions for probability generating function and by the use of method of moments). Different models are compared (more accurate nonlinear model and linear Lagergren model). The considerations are also done from the practical point of view (analyzing possibilities of reducing the influence of fluctuations on the operation of biosensors by controlling temperature and pressure, by adding controlled amounts of carrier analyte or by choosing the optimal timing for reading the output signal). Special attention is paid to the selection of the optimal procedure for computations with respect to detecting and preventing the spread of numerical errors.