# Finite Element Analysis Of A Bipolar-Electrochemistry Based Water Sensor

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## Abstract

This work computationally characterizes a new bipolar electrochemical sensing scheme recently developed for inexpensive detection of heavy metals in water. The sensing scheme employs a two-step optical anodic strip voltammetry protocol that couples a closed bipolar electrochemical cell with an electrochemiluminescent("ecl") reporter for quantification thereby avoiding expensive potentiostatic circuitry. Device operation is straightforward, but the specific chemical, physical, and electrochemical parameters that govern device functioning are yet to be determined.

This study employees COMSOL Multiphysics® to construct a finite element model of the device for more systematic study. With the Electrochemistry Module and a 2D Geometry, a Secondary Current Distribution physics interface is used to determine current density at both bipolar electrode("bpe") and electrolytes, as well as the potential drop (versus adjacent reference) across the whole system and across the BPE. A two-step time dependent study was employed to determine these variables at the first platting step, and utilizing the values of the first step as the initial value for the stripping step the same variables were assessed at the optical event (the ECL emission). Additionally, electrode deformation (given the deposition of a species of interest) and some of its effects were modelled by coupling the Transport of Dilute Species physics interface. Chemical processes of dilute species were also incorporated into the model and its impact on the design and functioning was assessed. Some factors that affect the position of the line of zero potential (LZP) were determined, such as relative conductivity of electrolytes and relative exposed area of the bipolar electrode. Additionally, some alternative geometries and sizes were explored as well as the effect of pH on the overall system. The model, although limited, sheds light to the main aspects that must be considering when designing and working with closed-cell bipolar electrodes as electrochemical sensors.

## Figures used in the abstract

**Figure 1** : Overall sensing scheme and calibration curve for ECL reporting mechanism.

**Figure 2** : 2D Approximation of proposed sensing scheme utilized for Multiphysics model. Note a single electrode (middle rectanle) is polarized to act as both a cathode and anode at its different ends.