Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information: Enhanced gold nanoparticle chemiresistor response to low-partitioning organic analytes induced by pre-exposure to high partitioning organics

Karl-Heinz Müller, Nereus Patel, Lee J. Hubble, James S. Cooper and Edith Chow
CSIRO Manufacturing, Lindfield, NSW, 2070, Australia

Limit of Detection

Using the octane pre-exposure method to enhance the gold nanoparticle film chemiresistor response only works for analytes with sufficiently small P. For the current enhancement factor F to be greater than 1, for small analyte concentration c_m, one obtains the following constraint on P_m

$$P_m(0) + P_m(1) \; < \; c_o P_o(0) \;\; [\, \ln P_o(0) - \ln P_o(1) \,] \;\; . \tag{15}$$

With a maximum assumed value of $c_o P_o(0) \approx 0.3$, one finds

$$P_m(0) + P_m(c_o) \;\lesssim\; 2.3 \;\; . \tag{16}$$

Therefore, in order for the pre-exposure method to work, the analyte partition coefficient has to be sufficiently small.

The question then arises as to what is the minimum detectable analyte concentration c_m?

Without pre-exposure to octane, *i.e.* $c_o = 0$, the gold nanoparticle chemiresistor current response to a small analyte concentration is (from Eq. (12))

$$\frac{\Delta I}{I}|_{c_o \,=\, 0} = -\beta L \; c_m \; P_m(0) \;\; . \tag{17}$$

With pre-exposure to octane, *i.e.* $c_o \neq 0$, the chemiresistor current response is obtained by multiplying the right hand side of Eq. (17) by $F(c_m \to 0)$ of Eq. (12). One obtains

$$\frac{\Delta I}{I}|_{c_o \neq 0} = \beta L_0 \; c_m \; [c_o P_o(0) \; (\ln P_o(0) - \ln P_o(1)) - P_m(c_o)] \;\; . \tag{18}$$

It is important to note that in contrast to Eq. (17), Eq. (18) is no longer proportional to $P_m(0)$. Assuming $\beta L = 10$, $P_m(c_o) \ll 1$ and that the experimental instrumentation has at best a current resolution of 10^{-5}, one finds in the case of 2 ppm octane pre-exposure $c_o P_o(0) \approx 0.057$ and thus the minimal detectable analyte concentration is

$$(c_m)_{min} \approx 2.3 \text{ ppm} \;\; . \tag{19}$$

This is a number which is essentially independent of the kind of analyte as long as $P_m(c_o) \ll 1$. In contrast, in the case of methanol with $P_m(0) = 0.01$, without pre-exposure to octane, using Eq. (19), one would only achieve a detection limit $(c_m)_{min} \approx 100$ ppm.