Supplementary material

Detection limits of chemical sensors: applications and misapplications

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Derivation of equation (11)

Starting from eq (10)

$$x_C^2 = \frac{t^2 s_y^2}{r^2}\left(\frac{1}{k} + \frac{x_{LOD}^2 n}{D} + \frac{\sum x_i^2}{D} - \frac{2x_{LOD}\sum x_i}{D}\right)$$

$$0 = \frac{t^2 s_y^2}{r^2}\left(+x_C^2\left(\frac{n}{D} - \frac{r^2}{t^2 s_y^2}\right) - x_{LOD}\frac{2\sum x_i}{D} + \frac{1}{k} + \frac{\sum x_i^2}{D}\right)$$

$$0 = x_C^2\left(n - \frac{Dr^2}{t^2 s_y^2}\right) - x_C 2\sum x_i + \frac{D}{k} + \sum x_i^2$$

$$x_{C,1,2} = \frac{1}{2\left(n - \frac{Dr^2}{t^2 s_y^2}\right)}\left(2\sum x_i \pm \sqrt{\left(2\sum x_i\right)^2 - 4\left(n - \frac{Dr^2}{t^2 s_y^2}\right)\left(\frac{D}{k} + \sum x_i^2\right)}\right)$$

$$x_{C,1,2} = \frac{t^2 s_y^2}{nt^2 s_y^2 - Dr^2}\left(\sum x_i \pm \sqrt{\left(\sum x_i\right)^2 - n\frac{D}{k} + \frac{D^2 r^2}{kt^2 s_y^2} - n\sum x_i^2 + \frac{Dr^2}{t^2 s_y^2}\sum x_i^2}\right)$$

With eq (6)

$$D = n\sum x_i^2 - \left(\sum x_i\right)^2$$

We insert…

$$x_{C,1,2} = \frac{t^2 s_y^2}{nt^2 s_y^2 - Dr^2}\left(\sum x_i \pm \sqrt{-n\frac{D}{k} + \frac{D^2 r^2}{kt^2 s_y^2} + \frac{Dr^2}{t^2 s_y^2}\sum x_i^2 - D}\right)$$

… and rearrange

$$x_{C,1,2} = \frac{ts_y}{nt^2 s_y^2 - Dr^2}\left(ts_y\sum x_i \pm \sqrt{\frac{D^2 r^2}{k} + Dr^2\sum x_i^2 - n\frac{D}{k}t^2 s_y^2 - Dt^2 s_y^2}\right)$$

With $x_{LOD} = 2\, x_C$ we obtain equation (11)

$$x_{LOD} = \frac{2ts_y}{nt^2 s_y^2 - Dr^2}\left(ts_y\sum x_i \pm \sqrt{\frac{D^2 r^2}{k} + Dr^2\sum x_i^2 - n\frac{D}{k}t^2 s_y^2 - Dt^2 s_y^2}\right) \qquad (11)$$

This has to be compared to the equation (4.19) in the article by Currie and Svehla [reference 4] which can be rearranged to give equation (14)

$$x_{LOD} = \frac{2t\sqrt{s_a^2+s_y^2}}{b}\frac{1-\frac{\sum x_i}{\sqrt{n\sum x_i^2}}\frac{s_a}{\sqrt{s_a^2+s_y^2}}t\frac{s_b}{b}}{1-t^2\frac{s_b^2}{b^2}} \qquad (14)$$

After rewriting equation (14) we obtain

$$x_{LOD} = \frac{\frac{2t\sqrt{s_a^2+s_y^2}}{b}-\frac{2t\sqrt{s_a^2+s_y^2}}{b}\frac{\sum x_i}{\sqrt{n\sum x_i^2}}\frac{s_a}{\sqrt{s_a^2+s_y^2}}t\frac{s_b}{b}}{1-t^2\frac{s_b^2}{b^2}}$$

$$x_{LOD} = \frac{2t\,b\sqrt{s_a^2+s_y^2}-2t^2\frac{\sum x_i}{\sqrt{n\sum x_i^2}}s_a s_b}{b^2-t^2 s_b^2}$$

The variable names are different from Harris (ref [6] of the main article) and the names used in the article and we identify:

- sensitivity: $b \rightarrow r$
- uncertainty of the sensitivity: $s_b \rightarrow s_r$
- uncertainty of the intercept: $s_a \rightarrow s_b$

We therefore rewrite using our names

$$x_{LOD} = \frac{2t\,r\sqrt{s_b^2+s_y^2}-2t^2\frac{\sum x_i}{\sqrt{n\sum x_i^2}}s_b s_r}{r^2-t^2 s_r^2}$$

Insertion of equations (7)…

$$s_r = s_y\sqrt{\frac{n}{D}}; \qquad s_b = s_y\sqrt{\frac{\sum x_i^2}{D}} \qquad (7)$$

…gives:

$$x_{LOD} = \frac{2t\,r\sqrt{s_b^2+s_y^2}-2t^2\frac{\sum x_i}{\sqrt{n\sum x_i^2}}s_b s_r}{r^2-t^2 s_r^2}$$

$$x_{LOD} = \frac{2t\,r\sqrt{s_y^2\frac{\sum x_i^2}{D}+s_y^2}-2t^2\frac{\sum x_i}{\sqrt{n\sum x_i^2}}s_y\sqrt{\frac{\sum x_i^2}{D}}s_y\sqrt{\frac{n}{D}}}{r^2-t^2 s_y^2\frac{n}{D}}$$

$$x_{LOD}=\frac{2t\,rs_y\sqrt{\frac{\sum x_i^2}{D}+1}-2t^2\sum x_i\ {}_y\,\frac{s_y^2}{D}}{r^2-t^2s_y^2\,\frac{n}{D}}$$

$$x_{LOD}=\frac{2t\,rs_y\sqrt{D\sum x_i^2+D^2}-2t^2\,s_y^2\sum x_i}{Dr^2-t^2s_y^2n}$$

$$x_{LOD}=\frac{2ts_y}{Dr^2-t^2s_y^2n}\left(r\sqrt{D\sum x_i^2+D^2}-t\,s_y\sum x_i\right)$$

And finally equation (15)

$$x_{LOD}=\frac{2ts_y}{nt^2s_y^2-Dr^2}\left(t\,s_y\sum x_i-\sqrt{Dr^2\sum x_i^2+r^2D^2}\right) \tag{15}$$

This may be compared to eq (11) in the article

$$x_{LOD}=\frac{2ts_y}{nt^2s_y^2-Dr^2}\left(ts_y\sum x_i\pm\sqrt{\frac{D^2r^2}{k}+Dr^2\sum x_i^2-n\frac{D}{k}t^2s_y^2-Dt^2s_y^2}\right) \tag{11}$$

The expressions are identical aside from the term

$$\Delta=-Dt^2s_y^2\left(n/k+1\right) \tag{16}$$

as was discussed in appendix I of the main article.