Uncertainty in fatty acid methyl ester
Reference material characterization

Camilo D Aleman, Yolby M. Rodriguez & Immer M. Caicedo
Mol Labs Quimiométricas
quimiometria@mollabs.com

The usual uncertainty estimation from the EURACHEM Guide CG04 applied to assigned values of fatty acids for an edible oil CRM to be accredited, results in low values compared to the reference, a higher hierarchy material used for calibration (MRC DMR 528a CENAM). So, we use the model for uncertainties associated with the $x_i$ and the $y_i$, from the ISO/TS 28037:2010. Here we show detailed data for oleic acid and final results for our (finally !) accredited CRM.

Model: EURACHEM/CITAC CG04 Appendix E.4. linear least squares
The mathematical modeling was defined as:

$$\bar{Y} = \beta_0 + \beta_1 x_i$$

The regression for oleic acid showed results:

$$\bar{Y} = 125.68 + 5068.14 x_i$$

The calculation of the uncertainty $u(c_0)$ associated with the linear least square is estimated as:

$$u(c_0) = \sqrt{\frac{S}{\hat{B}_1} \hat{B}_1 + \frac{1}{n} \left( \frac{\bar{c}_0 - \bar{c}}{s_x} \right)^2}$$

Model: ISO/TS 28037:2010 chapter 7. Uncertainties associated with the $x_i$ and the $y_i$
The case corresponds to that described by the statistical model:

$$x_i = X_i + d_i \quad y_i = Y_i + e_i \quad Y_i = A' + B'X_i, \quad i = 1, \ldots, m$$

With,

$$a = \left[ \begin{array}{c} -526.62 \\ 5234.02 \end{array} \right] \quad u = \left[ \begin{array}{c} 23427.96 \\ -8704.66 \end{array} \right]$$

The mathematical modeling was defined as:

$$\bar{Y} = \beta_0 + \beta_1 x_i$$

The regression for oleic acid showed results:

$$\bar{Y} = 125.68 + 5068.14 x_i$$

Final results

### Table 1- Assigned value $g$ 100 g$^{-1}$ and uncertainty for all characterized fatty acids

<table>
<thead>
<tr>
<th>Fatty Acid</th>
<th>Assigned Value</th>
<th>Uncertainty ($u$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stearic acid</td>
<td>2.16</td>
<td>$U_k=0.12$</td>
</tr>
<tr>
<td>Palmitic acid</td>
<td>4.32</td>
<td>$U_k=0.19$</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>15.01</td>
<td>$U_k=0.59$</td>
</tr>
<tr>
<td>Oleic acid</td>
<td>45.7</td>
<td>$U_k=1.7$</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>$U_k=3.6$</td>
</tr>
</tbody>
</table>

Conclusions:

• $R$ and Excel calculations for uncertainties associated with the $x_i$ and the $y_i$, are easy to compute. So, it will be safe and effective to use them: same results of linear least squares for negligible $x_i$ contributions.

References:


Acknowledgements:

- EMA Mexican accreditation body