CEToolbox Equations

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1 CEToolbox

The CEToolbox application[1] is a calculator for capillary electrophoresis[2]. It permits to calculate several parameters of a capillary electrophoresis analysis, like the hydrodynamic injection, the volume of the capillary, the quantity of injected analyte or the electroosmotic mobility.

This document presents the theoretical equations used by CEToolbox. For questions or remarks, please contact us through the CEToolbox project website.

2 Equations

2.1 Hydrodynamic injection

The volume of injected sample (nL) is calculated following the Poiseuille's law[3]:

$$V_{inj} = \frac{\pi d_c^4 t \Delta P}{128 \eta L} \times 10^{12}$$

where d_c is the internal diameter of the capillary (m), t the time to window (s), ΔP the applied pressure (Pa), η the viscosity (cP) and L the total length of the capillary (m).

2.2 Capillary volume

The volume of the capillary (nL) is computed accordingly to:

$$V_{tot} = \frac{\pi d_c^2 L}{4} \times 10^{12}$$

where d_c is the internal diameter of the capillary (m) and L the total length of the capillary (m).

2.3 Capillary volume to window

The capillary volume to detection window (nL) is determined with:

$$V_d = \frac{\pi d_c^2 l}{4} \times 10^{12}$$

where d_c is the internal diameter of the capillary (m) and l the length to detection window (m).

2.4 Injection plug length

The injection plug length (mm) is calculated with the following formula:

$$l_{inj} = \frac{4 V_{inj}}{\pi d_c^2} \times 10^{-9}$$

where V_{inj} is the volume of sample injected (nL) and d_c is the internal diameter of the capillary (m).

2.5 Plug

The percentage of plug is the ratio between the volume of injected sample and the capillary volume:

$$\%_{tot} = \frac{V_{inj}}{V_{tot}} \times 100$$

where V_{inj} is the volume of sample injected (nL) and V_{tot} the volume of the capillary (nL).

2.6 Plug relative

The percentage of relative plug is the ratio between the volume of injected sample and capillary volume to window:

$$\%_d = \frac{V_{inj}}{V_d} \times 100$$

where V_{inj} is the volume of sample injected (nL) and V_d the capillary volume to window (nL).

2.7 Time to replace one volume

The time (s) to replace one volume is computed with the following equation, obtained by combining the capillary volume and the hydrodynamic injection equations:

$$t = \frac{32\eta L^2}{d_c^2 \Delta P} \times 10^{-3}$$

where η is the viscosity (cP), L the total length of the capillary (m), d_c the internal diameter of the capillary (m) and ΔP the applied pressure (Pa).

2.8 Injection flow rate

The injection flow rate (nL/ min) is calculated with:

$$Q_{inj} = \frac{V_{tot}}{t}$$

where V_{tot} is the volume of the capillary (nL) and t the time (min).

2.9 Electrical field

The electrical field ($\mathrm{V\,cm^{-1}}$) is determined by:

$$E = \frac{U}{L} \times 10^{-2}$$

where U the voltage (V) and L the total length of the capillary (m).

2.10 Analyte injected

The quantity of injected analyte (ng) is computed with:

$$m = CV_{inj}$$

where C is the concentration (g/L) and V_{inj} the volume of injected sample (nL).

2.11 Electroosmotic mobility

The electroosmotic mobility ($\mathrm{m^2\,V^{-1}\,s^{-1}}$) is the ratio between the electrophoretic velocity and the electrical field:

$$\mu_{eof} = \frac{lL}{t_{eof}U}$$

where l is the length to detection window (m), L the full length of the capillary (m), t_{eof} the electroosmosis time (s) and U the voltage (V).

2.12 Separation flow rate

The separation flow rate ($\mathrm{nL\,min^{-1}}$) is determined with the formula:

$$Q_{sep} = \frac{\pi d_c^2 \mu_{eof} E}{4} \times 60 \times 10^{14}$$

where d_c is the inner diameter (m), E the electrical field ($\mathrm{V\,cm^{-1}}$) and μ_{eof} the electroosmotic mobility ($\mathrm{m^2\,V^{-1}\,s^{-1}}$).

2.13 Viscosity

The viscosity (cP) is computed with:

$$\eta = \frac{d_c^2 t_m \Delta P}{32 l L} \times 10^3$$

where d_c is the inner diameter (m), t_m the migration time (s), ΔP the applied pressure (Pa), l the length to detection window (m) and L the full length of the capillary (m),

2.14 Conductivity

The conductivity ($\mathrm{mS\,m^{-1}}$) is calculated with the formula[4]:

$$\kappa = \frac{4IL}{\pi d_c^2 U} \times 10^3$$

where I is the electric current (A), L the full length of the capillary (m), d_c the inner diameter (m) and U the voltage (V).

2.15 effective mobility

The effective mobility ($\mathrm{m^2\,V^{-1}\,s^{-1}}$) reprents the mobility of the compound wihtout taking into consideration the electroosmotic flow. It is calculated with the equation:

$$\mu_{eff} = \frac{lL}{t_m U} - \mu_{eof}$$

where l is the length to detection window (m), L the full length of the capillary (m), t_m the migration time (s), U the voltage (V) and μ_{eof} the electroosmosis mobility ($\mathrm{m^2\,V^{-1}\,s^{-1}}$).

References

[1] Y. François and J. Pansanel. CEToolbox v1.4.5, March 2021. URL `https://doi.org/10.5281/zenodo.4643845`.

[2] C. F. Poole. *Capillary Electromigration separation methods*. Elsevier, 2018.

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[4] Y. François, K. Zhang, A. Varenne, and P. Gareil. New integrated measurement protocol using capillary electrophoresis instrumentation for the determination of viscosity, conductivity and absorbance of ionic liquid–molecular solvent mixtures. *Analytica Chimica Acta*, 562(2):164–170, 2006. URL `https://doi.org/10.1016/j.aca.2006.01.036`.