

Developed by Víctor González-Ruiz, with the contribution of Nicolas Drouin, Emilie Reginato, Serge Rudaz and Julie Schappler

*Chimie Analytique Pharmaceutique, Section des Sciences Pharmaceutiques
Faculté des Sciences, Université de Genève*

This calculator is intended to be a handy tool for CE practitioners in every field. It will use the experimental conditions provided by the user to automatically calculate several characteristics of the hydrodynamic injection.

The screen is divided into three parts (fig. 1):

- “Experimental conditions” panel: allows the user to input the experimental parameters by using the numeric fields and choosing the adequate options within the drop-down menus.
- “Calculated parameters” panel: will display the computed values (the output units for some of them can also be selected by the user).
- The capillary graph on the lowest part will show a schematic representation of the parts of the capillary occupied by the different fractions.

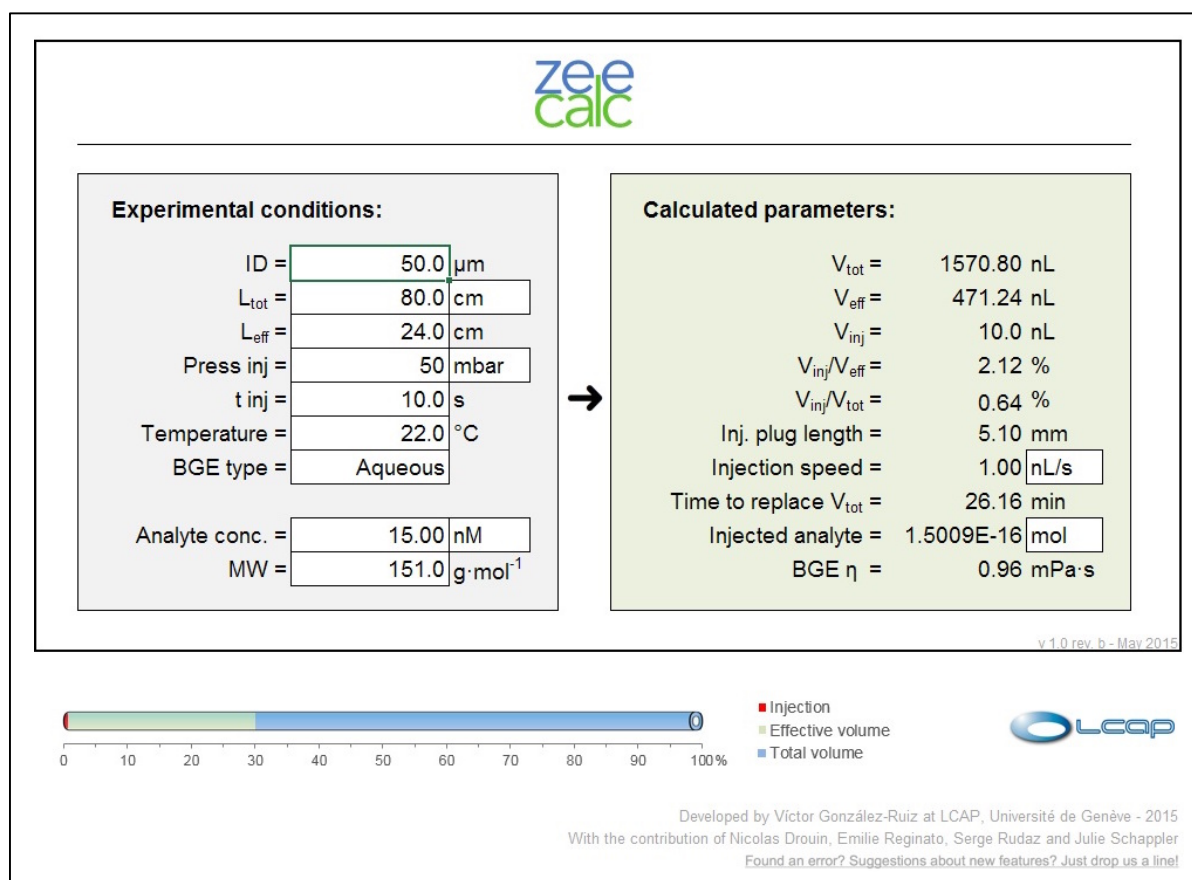


Figure 1.- Screenshot of zee calc showing the main three elements of its interface.

a) “Experimental conditions” panel:

a.1) Capillary

The total (“ L_{tot} ”) and effective (“ L_{eff} ”) lengths of the capillary can be typed down in cm or inches. The inner diameter “ ID ” must be specified in μm .

a.2) Injection

The hydrodynamic injection can be defined by using the duration (“ $Time$ ”, in seconds) and the applied pressure (“ $Press\ inj.$ ”, in mbar or psi).

a.3) BGE

The drop-down menu “ $BGE\ type$ ” allows the user to select the composition of the BGE in order to calculate its viscosity. Four options are available: “Aqueous”, “Water:MeCN”, “Water:MeOH” and “User defined” (fig. 2).

Temperature =	22.0 °C	Temperature =	22.0 °C	Temperature =	22.0 °C
BGE type =	Aqueous	BGE type =	Water:MeCN	BGE type =	User defined
Analyte conc. =	15.00 nM	% MeCN =	10.00	BGE η =	10.00 mPa·s
		Analyte conc. =	15.00 nM	Analyte conc. =	15.00 nM

Figure 2.- zeecalc provides several options to automatically calculate the viscosity of the BGE. A personalized value can also be specified instead.

When “Aqueous” BGE is selected, the specified temperature will be considered in order to calculate the viscosity of the BGE.

If “Water:MeCN” or “Water:MeOH” are selected, the percentage of organic solvent present in the BGE must be specified either in the “% MeCN” or in the “% MeOH” field. This value, together with the temperature, will be employed to calculate the viscosity of the aqueous-organic mixtures.

The fourth option, “User defined”, can become useful when the calculations should be carried out considering a predefined viscosity value (for example, when the nature of the BGE is different from the three ones included in the utility). This value can be typed down in the field “ $BGE\ \eta$ ” (in mPa·s). No temperature correction is possible in this case, as the viscosity value will be used “as is”.

a.4) Sample

The concentration of the sample can be specified in the “ $Analyte\ conc.$ ” field. Different concentration units can be chosen within the options in the drop-down menu on the right (fig. 3). Molecular weight (“ MW ” field) will be used if molar and mass concentrations are simultaneously used in the input and output panels. If only molar or only mass concentrations are employed, the value in this field will not be considered.

BGE η =	10.00	mPa·s
Analyte conc. =	15.00	nM
MW =		M mM μ M nM <u>μg/mL</u> ng/mL

Time to replace V_{tot} =	26.16	min
Injected analyte =	1.5009E-16	mol mmol μ mol nmol pmol ng <u>pg</u>
BGE η =	0.96	

Figure 3.- “Sample concentration” and “Injected amount” fields showing the several available units.

b) Output panel

The volume of the injection is calculated by means of Poiseuille’s equation (eq. 1).

$$V_{inj} = \frac{\Delta P d^4 \pi t_{inj}}{8 \eta l} \quad (1)$$

If not defined by the user, the viscosity is calculated –according to the nature of the BGE and to the temperature– by applying one of the following equations (eqs. 2–4):

$$\text{Water} \quad \eta_T = 2.414 \cdot 10^{-2} \text{ mPa}\cdot\text{s} \cdot 10^{247.8 \text{ K}/(T-140 \text{ K})} \quad (2)$$

$$\text{Water:MeOH} \quad \eta_{\Phi_{\text{MeOH}}, T} = 10^{(-2.429+(714/T)-1.859\Phi+(911.7\Phi/T)+1.8586\Phi^2-968.1(\Phi^2/T))\text{K}} \text{ mPa}\cdot\text{s} \quad (3)^*$$

$$\text{Water:MeCN} \quad \eta_{\Phi_{\text{MeCN}}, T} = 10^{(-2.063+(601.9/T)+0.0709\Phi+(62\Phi/T)+0.5043\Phi^2-345.8(\Phi^2/T))\text{K}} \text{ mPa}\cdot\text{s} \quad (4)^*$$

*Eqs. 3 and 4 taken from D. Guillarme, S. Heinisch, J.L. Rocca, *J. Chrom. A*, 1052 (2004) 39–51

The injection speed can be displayed in nL/s or nL/min, and the units used to show the injected amount of analyte can be chosen from the drop-down menu on the right (fig. 3).

c) Capillary graph

This graph will dynamically display the volumes of the capillary corresponding to the injected plug, the effective volume and the total volume (fig 4). Every colour bar should be read as starting at the 0% position. For example, if the red bar corresponding to the injected volume represents the 2% of the capillary, and the green V_{eff} bar reaches the 20% mark, it means that the V_{eff} corresponds to a 20% of the capillary volume, *not* to a 18% (20%-2%).

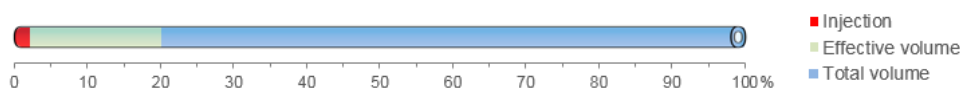


Figure 4.- The capillary graph shows the percentage of the total volume corresponding to the sample plug and the effective length.

If you found this calculator useful to your work, please cite this electronic resource as:

V. González-Ruiz, N. Drouin, E. Reginato, S. Rudaz and J. Schappler. “zeecalc 1.0”, available online at <https://epgl.unige.ch/labs/fanal/zeecalc>