

Application Note AN-DV-001

化学和光学果理的 DropView 解决方案

Four key software tools for curves data processing and analysis

Electrochemistry, spectroscopy, and spectroelectrochemistry (SEC) are widely used techniques in many fields. However, the data curves obtained from these analyses are quite varied, and not all electrochemical peaks and spectroscopic bands can be measured with the same procedures.

This Application Note reveals four tools included in the DropView 8400 and DropView SPELEC

softwares to facilitate the measurement and analysis of the collected curves and data. The selection of the appropriate procedure can help the measurement process and thus facilitate the analysis of the results.

The following measurement options are explained in detail: automeasurement, set on curve measurement, set free measurement, and set step measurement.

INSTRUMENTATION AND SOFTWARE

The curves shown in this study have been obtained with SPELEC and a μ Stat 400 instrument controlled by DropView SPELEC and DropView 8400 software, respectively.

The SPELEC is a fully integrated instrument available for electrochemical, optical, and spectroelectrochemical measurements in several different spectral ranges. The μ Stat 400 in strument is a portable bipotentiostat/galvanostat.

DropView SPELEC is an advanced and dedicated software that acquires spectroelectrochemical data in real time and includes specific tools for data processing and analysis. The DropView 8400 software provides the electrochemical responses and includes different tools for data processing.

In the following sections, different tools for measuring electrochemical and spectroscopic signals will be elucidated exhaustively.

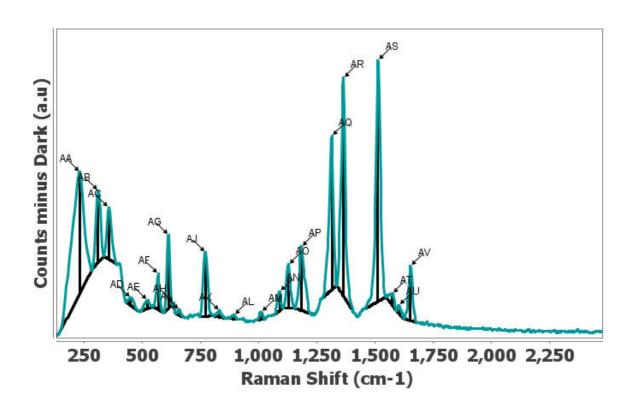
RESULTS AND DISCUSSION

Four of the tools available in the DropView 8400 and DropView SPELEC softwares have been implemented to perform measurements on electrochemical and spectroscopic curves as shown below:

Automeasurement (software icon)

This tool is suitable for automatic measurements on a curve. Using this tool is as easy as selecting the electrochemical or spectroscopic curve on which it is to be applied and then selecting the *automeasurement* tool.

Figure 1 shows the result of the measurement of a Raman spectrum using the automeasurement tool. Moreover, as shown in the figure, this tool recognizes all of the bands and displays the information associated with each Raman signal.



AQ
Height: 600.683 counts (a.u.)
Width: 20.867 cm-1
Peak position: 1314.495 cm-1
Area: 23773.278 counts (a.u.)*cm-1
Peak Area: 13055.26 counts (a.u.)*cm-1
Start: 1272.568 cm-1
End: 1335.304 cm-1
AR
Height: 852.339 counts (a.u.)
Width: 20.619 cm-1
Peak position: 1364.853 cm-1
Area: 29397.476 counts (a.u.)*cm-1
Peak Area: 18843.652 counts (a.u.)*cm-1
Start: 1335.304 cm-1
End: 1408.79 cm-1

Figure 1. Raman spectrum measured by the automeasurement default tool and the information related to AQ and AR bands.

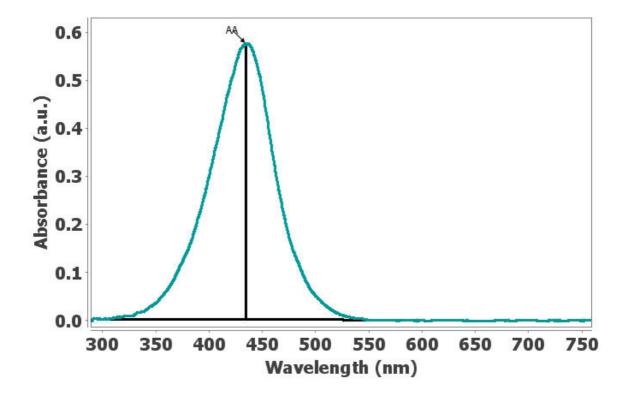
In addition, in **Figure 1**, numerous bands can be perceived in the spectroscopic curve, but the *automeasurement* tool offers a quick procedure to obtain the information associated with all peaks, instead of needing to manually measure each band on its own.

Furthermore, the default settings of this tool can be modified to optimize the automatic measurement according to the shape of the selected curve.

Set on curve measurement (software icon)

This option allows users to measure the peak between two selected points on the curve. It is not necessary to precisely define these two points, as the tool will automatically search for the point on the curve closest to the area that has been selected.

In Figure 2, a straight line is drawn between the two selected points (300 nm and 550 nm) and a vertical line is created where the height is equal to the maximum value of the UV/VIS band.





Height: 0.574 a.u. Width: 65.367 nm

Peak position: 434.666 nm Area: 43.024 a.u.*nm

Peak Area: 42.61 a.u.*nm

Start: 298.527 nm End: 570.532 nm

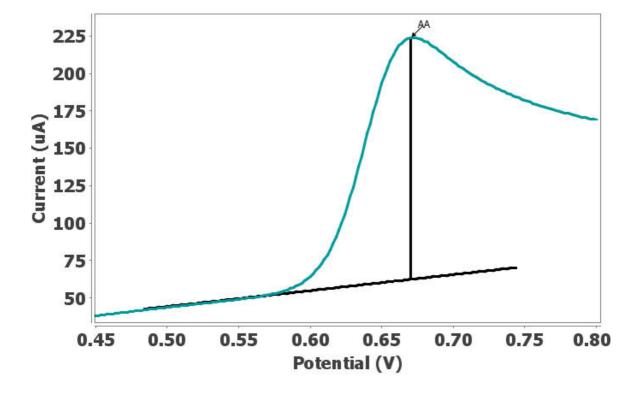
Figure 2. UV/VIS band measured by set on curve measurement tool and the related information shown for this absorption band.

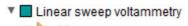
Set free measurement **△** (software icon)

Set free measurement performs in a similar manner to the case of the set on curve measurement tool, but differs in that the selected points are not automatically adjusted to the nearest points on the curve. Therefore, these

two points must be precisely defined when using the *set free measurement* tool.

In **Figure 3**, the oxidation peak has been measured in a linear sweep voltammogram considering the correction of the initial capacitive current.





Height: 161.257 uA

Width: 0.11 V

Peak position: 0.67 V

Charge (Peak): 804.143 uC

Area: 30.745 uA*V Peak Area: 16.083 uA*V

Start: 0.484 V End: 0.744 V

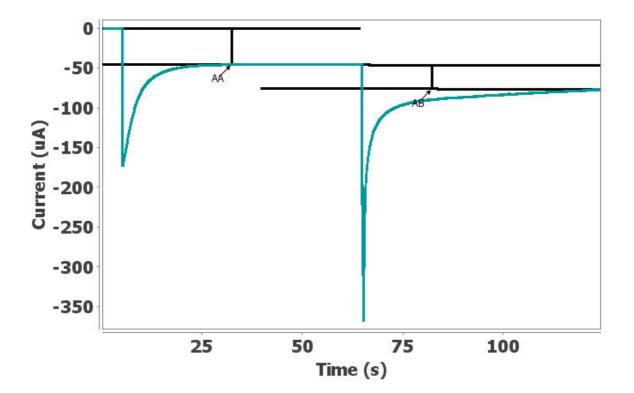
Figure 3. Measurement of oxidation peak by the set free measurement tool in a linear sweep voltammogram, including the information related to this anodic peak.

Set step measurement (software icon)

Suitable for measuring «steps», the set *step measurement* tool allows users to select three main points on the curve to measure. To mark the first point, the closest point on the selected curve will be taken, just as with the *set on curve measurement* tool. In contrast, the next two points must be selected accurately, just as with

the set free measurement tool.

As shown in **Figure 4**, the *set step measurement* is applied to the electrochemical response obtained by a multipulsed amperometric detection procedure. This tool draws a straight baseline between the first two selected points, while the third point defines a parallel line with respect to the baseline.





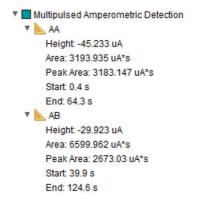


Figure 4. Measurements performed by the set step measurement tool after multipulsed amperometric detection, showing the information obtained for this analysis.

CONCLUSION

The DropView 8400 and DropView SPELEC softwares are specific solutions for monitoring electrochemical processes and, in the latter case, also optical and spectroelectrochemical events. In addition, they offer advanced tools for data processing and analysis.

This Application Note has explained how to use four of these tools that are focused on the measurement of electrochemical and optical curves, accompanied by specific examples. The selected options discussed include: automeasurement, set on curve measurement, set free measurement, and set step measurement.

These different procedures allow users to select the tool that provides the most accurate measurement of the curves for each in dividual case.

CONTACT

瑞士万通中国 北京市海淀区上地路1号院 1号楼7702 100085 北京

marketing@metrohm.co



CONFIGURATION



SPELEC UV-VIS 200-900 nm

SPELEC 是一行光化学量的器。SPELEC 将一个光源、一个双恒位/恒流和一个光(UV/VIS 波范:200-900 nm)合在一个箱子中,并配有用的光化学件,可同步行光学和化学。

