

Quality control of chemical measurements

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The practice of customer service in chemical measurements develops a need for quality control associated with three properties of such measures:

1. Intermediate precision (IP) in measurements, therefore,
2. A common IP uncertainty. And
3. Dissimilar values in real matrix measurements.

An alternative use of algorithms z -score and En from proficiency testing, allow to draw all the data to be used as internal quality control.

There are two kinds of central points in this quality control charts: 1. Replicates (r ●) and internal reference sample (rs ▲), measured in IP conditions. 2. Reference materials (CMR ■) and proficiency testing (PT *), measured in reproducibility conditions. But, their replicates can be treated as replicates. Then it is possible to draw a control chart.

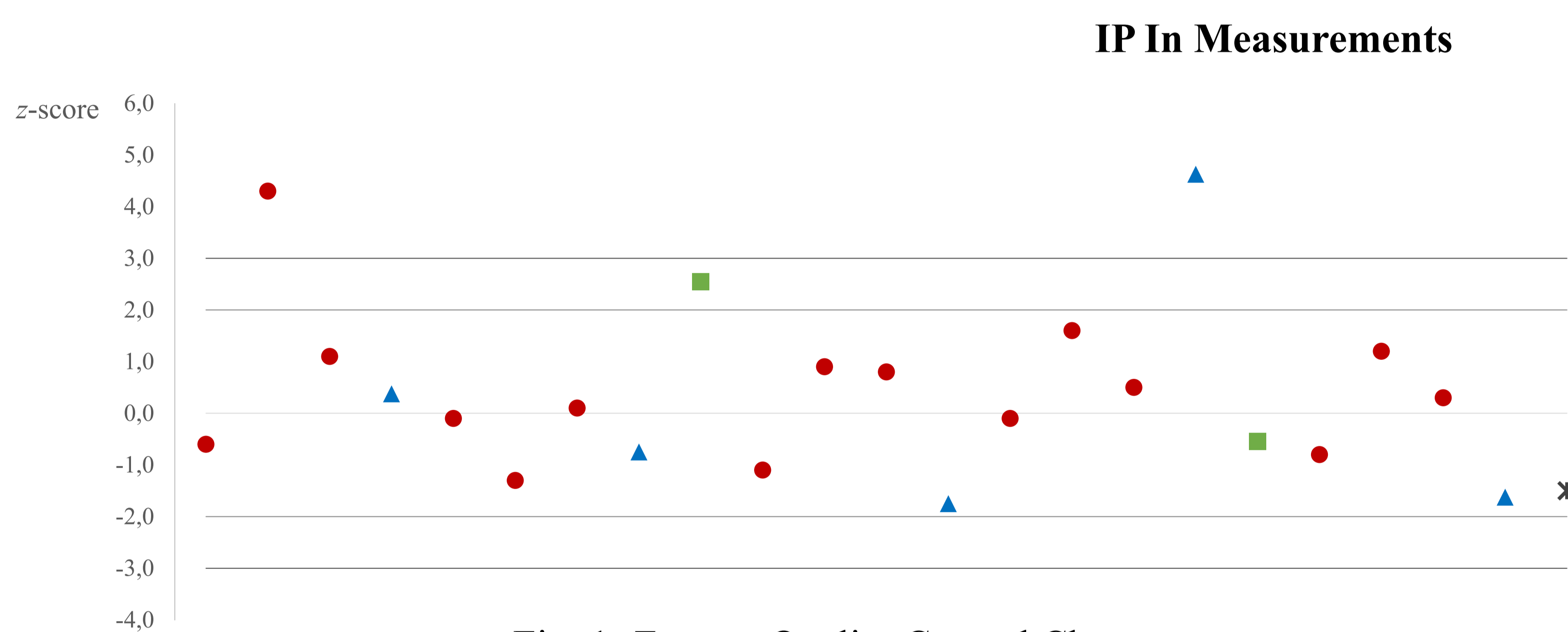


Fig. 1: Z-score Quality Control Chart.

$z\text{-score} = (x - X) / s$, will describe how much a point deviates from a mean or specification point., by the use of standard uncertainty $u_x = U/k$.

As example in fig 1, Iodine number in vegetable oils: mg I₂/100g. Procedure AOAC 920.169.

Internal validation standard, safflower oil; replicates Palm oil; CRM FAPAS oil, PT Sample from FAPAS also. All data from IP replicates.

As usual as it must be expected aleatory distribution of data points. Trends or non central distribution of data warns about procedure troubles and reflects procedure, materials or analyst changes, and or equipment malfunctions.

$En = (x - X) / (\sqrt{U_x^2 + U^2})$: By the use of expanded uncertainty U of the measurement in account. As example, same data on fig 1. looks as fig 2. Also it must be expected aleatory distribution of data points on central distribution. At least 95% of uncertainty lines must touch the central line, or uncertainty has a poor estimation. IP uncertainty must be smaller than the reproducibility one. Also if all data touch the central line, uncertainty has a larger estimation. Be careful of a chart with at least 30 data points.

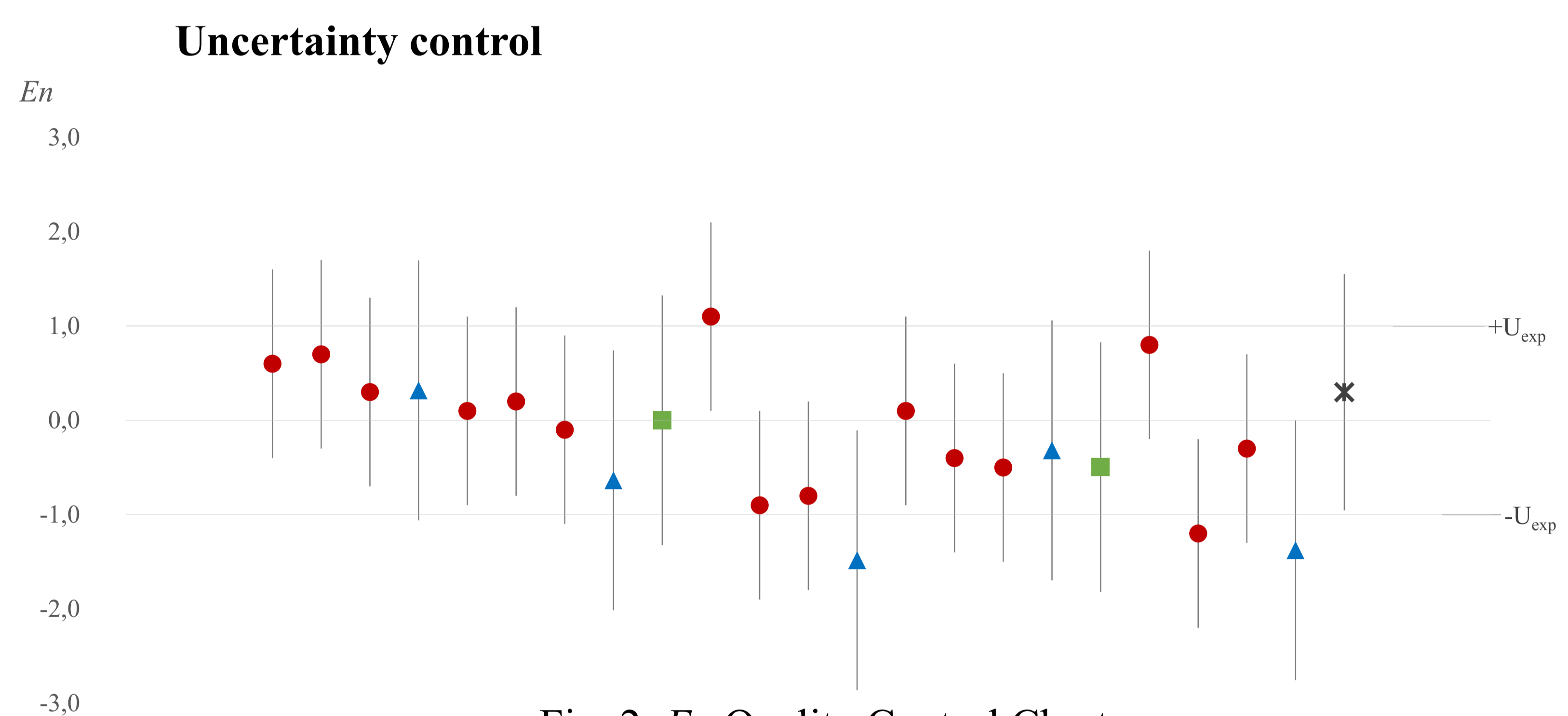


Fig. 2: En Quality Control Chart.

Uncertainty estimation could be controlled from this chart.

Conclusions

- 1 z -score and En quality control charts have advantage to integrate low medium or high of levels data measurement.
2. And few data points can be used to start adjusts in analytical procedures or uncertainty estimation.
3. But En has twice the information, one about central point and another on uncertainty.

Bibliography

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- [3] ASTM. "Manual on Presentation of Data and Control Chart Analysis". 7th Edition. February 2002.