QC Tools at Your Fingertips:

Utilizing Excel in QC analysis, tracking, evaluation, and reporting

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We already know we're good, so why do we need this again?

- Effective internal QC program involves a continuous, critical evaluation of the analytical process, from log-in to reporting
- The QC has to be part of a quality system and should be formally reviewed on a regular basis.
- Allows you to recognize, quantitate, and minimize errors.
- Describes and documents the accuracy and precision of the data.

Values of an Effective QC Program

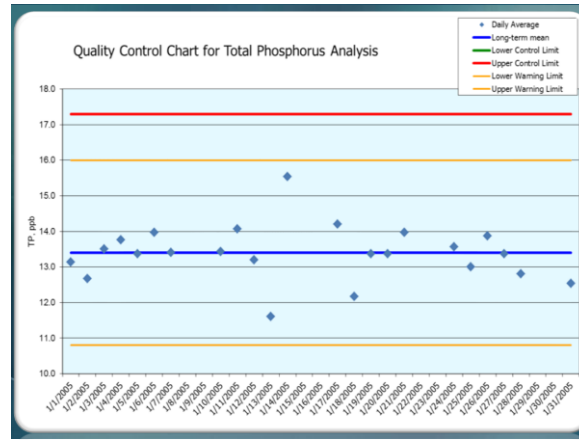
- Important quality tool for the analysts
- Important continuous audit of analytical process for management
- Reporting analytical quality to customers or potential clients
- Documentation of quality for legal defensibility purposes
- Estimation of the measurement uncertainty

Important Components of a Quality Control Program

- Preparation and analysis of QC at the level and frequency required by NELAC and the reference methodology
- Quality control charting
- Proficiency testing
- the participation in inter-laboratory comparisons (round robin programs)
- the use of certified reference materials
- method validation.

QC Charts (X-bar charts)

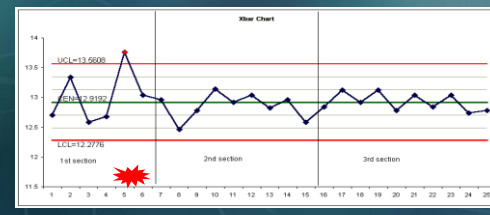
- Control charting is a powerful and simple tool for the short-term and long-term QC of routine analytical process.
  - QC samples are analyzed routinely with the each sample batch. together with the routine samples in an analytical run.
    - Blanks, laboratory control samples, matrix spikes, replicates, certified reference materials
    - Blind samples
  - Immediately after the analytical run is completed the *control values* are plotted on a control chart.



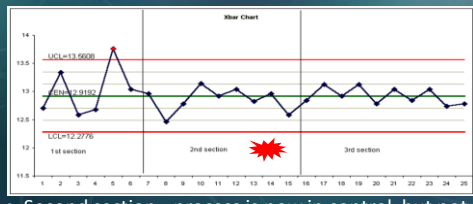
QC Chart Components

- **Central line (CL)**: represents the mean value over a period of time or over a number of analyses, or the nominal value of a certified reference material.
- **Warning limits**: ± 2 times the standard deviation from the central line (CL ± 2s); upper warning limit (**UWL**) and lower warning limit (**LWL**)
  - Assuming a normally distributed data, about 95 % of the results should fall within the warning limits.
- **Control limits**: ± 3 times the standard deviation from the central line (CL ± 3s); upper control limit (**UCL**) and lower control limit (**LCL**).
  - Also referred to as the action limits
  - 99.7 % of the data normally distributed should be within these limits. (Statistically, only 3 out of 1000 measurements are outside the action limits).

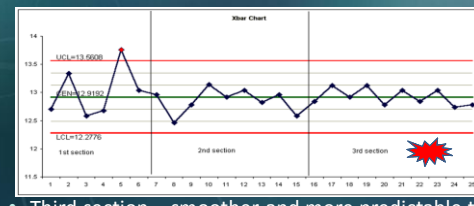
QC Chart Example



- First section – out of control
  - Wide range in fluctuation or results
  - one point is outside of the control limits
- Interpretation and action: There is a source of special random cause variation; root cause needs to be determined and resolved.



- Second section - process is now in control, but not quite smooth yet. Still have a couple of points at around the warning limits
- Interpretation and action: Likely some common cause variations. Needs to be investigated and resolved.



- Third section – smoother and more predictable trend.
  - Little variation, above and below the central line.
  - Evidence of process improvement
- Interpretation and action: Relax, pat yourself in the back.

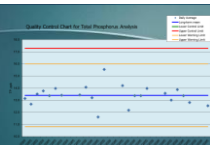
Examining the QC Charts

- **RUN** - When several plotted points line up consecutively on one side of a Central Line (CL), whether it is above or below the CL, it is called a "run". Seven points in a row on one side of the CL indicates an abnormality in the process and needs to be investigated and resolved.
- **TREND** - there is a continued rise or fall in a series of points (like an upward or downward slant). Usually indicates a process is drifting out of control. Likely due to analytical instrument drifting response or unstable chemical solution.
- **CYCLE** - plotted points show the same pattern of change over equal intervals. Could be an indicator of some systematic drift to both sides of the centerline.
- **HUGGING** - When the points on the control chart seem to stick close to the center line or to a control limit line. May need closer analysis.

How often should the control limits and central line be updated?

- If the method and instrument is working, the control limits and the central line remain stable over a long period of time.
- Should not be changed frequently since this will make it difficult to detect gradual changes in analytical quality.
  - Evaluate at least every year or after collection of ~20- 30 data points. Evaluation does not necessarily mean that the control limits should be changed.
  - A change should only be considered if a significant change in spread or the bias has taken place.
- The laboratory should have a policy for how often control limits are evaluated and updated.

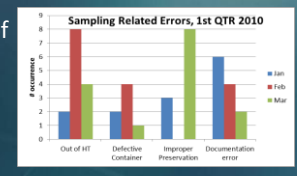
Creating QC Charts in Excel

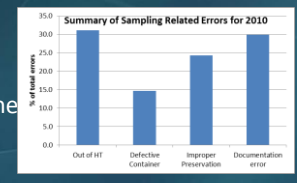


- Organize your data in column format
- Calculate the long-term mean and standard deviation
- Calculate 2- and 3-sigma values (std dev)
- Calculate warning and control limits
- Create a column with the mean value copied in the entire column (up to the last row with analytical QC result entry)
- Create column with LCL, UCL, LWL, and UWL values copied down the column
- Create a line graph for mean, UCL, LCL, LWL, and UWL

Tracking and analyzing categorical errors

- Allows us to visualize frequency distribution of categorical information.
  - Examples: errors in sampling, sample receiving, sample preparation
- Can be useful for management in determining improvement areas in the laboratory (or field sampling)





Using Excel to Plot and Analyze Categorical Data

- Create a spreadsheet for logging errors or defects
- Group errors into categories
- Obtain the sum of errors on monthly and yearly basis
- For each category, calculate % of total errors
- Use Excel's column or bar chart to plot

The 80/20 Rule: 20 percent of the defects causing 80 percent of the problems (Juran); 20 percent of the work consume 80 percent of your time and resources.

Evaluating laboratory result versus a single reference value

- Test for:
  - Null hypothesis:
  - Alternative hypothesis:
- Z-score (standardized test)
  - Use when you have a large data set (>30)
  - Assumption: normal data distribution
- One-sample t-test
  - Use when you have a smaller data set
  - Assumption: normal data distribution

Z-score

- How many standard deviation is our result from the study mean (or most probable value or true value)?

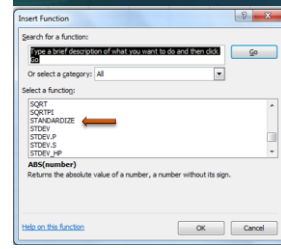
QC Type	Date of Study	Lab result	Study mean	Study Std Dev.	z-score
PT Study	1/12/2011	25.2	28.3	4.6	-0.674
Round robin study	3/25/2011	44.1	47.6	11.8	-0.297
Blind study	6/20/2011	11.4	10.1	6.2	0.210
PT Study	7/2/2011	35.7	39.2	15.6	-0.224

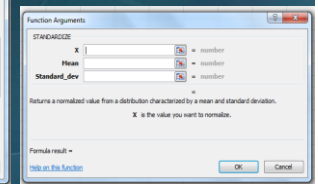
USGS' Use of Z-score (Z-value) to rate laboratories for their round robin studies.

Absolute Z-value	Rating
0.00 - 0.50	4 (Excellent)
0.51 - 1.00	3 (Good)
1.01 - 1.50	2 (Satisfactory)
1.51 - 2.00	1 (Marginal)
greater than 2.00	0 (Unsatisfactory)
	NR (Not Rated)

Using Excel to Generate Z-scores

- Use the "**Standardize**" function in Excel to obtain the Z-score.
- X will be your result, mean is the study mean (or true value), Standard dev is the study standard deviation.





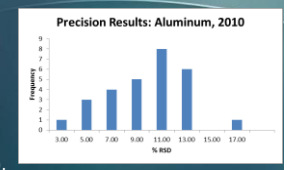
Summary Statistics

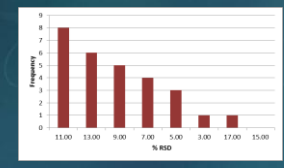
- data range (maximum value-minimum value)
- min/max
- central tendency (mean, median, mode)
- data variability (std dev, std error, variance)
- can easily calculate warning and control limits

Summary Statistics: Aluminum MS	
Mean	87.84285714
Standard Error	0.866233539
Median	88.6
Mode	82.4
Standard Deviation	3.969580762
Sample Variance	15.75757143
Kurtosis	-0.066924286
Skewness	-0.510597408
Range	15.9
Minimum	78.9
Maximum	94.8
Sum	1844.7
Count	21
2-sigma	7.939161525
3-sigma	11.90874229
LWL	79.9
UWL	95.8
LCL	75.9
UCL	99.8

Histograms

- A histogram, or frequency distribution chart, represents the distribution of data.
- Created by grouping data according to classses (called bins), count the number of data points that fall into each bin, and plotting the count, frequency, or percentage values.
- Y-axis represents the frequency, and the X- axis represents bins of data. It is also called a frequency distribution chart.





Comparing Two Methods Using T-test

- Can be independent or paired t-test, depending on relationship between the two data sets.
- Paired t-test - used to investigate the differences between two data sets where there is a meaningful one-to-one correspondence between the data points
  - Example: same field sample, analyzed twice: 1 using ICP-AES, and the other using ICP-MS.

$$t = \frac{d_{av}}{SD/\sqrt{N}}$$

- d_{av} is the mean difference, i.e. the sum of the differences of all the datapoints divided by the number of pairs
- SD is the standard deviation of the differences between all the pairs
- N is the number of pairs.
- The sign of t (+/-) does not matter, assume that t is positive.

Paired t-test (continued)

- If the calculated value of t is greater than the critical value, H_0 is rejected, i.e. there is evidence of a statistically significant difference between the groups.
  If the calculated value of t is less than the critical value, H_0 is accepted, i.e. there is no evidence of a statistically significant difference between the two groups.

t Table

cum. prob	$t_{.50}$	$t_{.75}$	$t_{.80}$	$t_{.85}$	$t_{.90}$	$t_{.95}$	$t_{.975}$	$t_{.99}$
one-tail	0.50	0.25	0.20	0.15	0.10	0.05	0.025	0.01
two-tails	1.00	0.50	0.40	0.30	0.20	0.10	0.05	0.02
df								
1	0.000	1.000	1.376	1.963	3.078	6.314	12.71	31.82
2	0.000	0.816	1.061	1.386	1.886	2.920	4.303	6.965
3	0.000	0.765	0.978	1.250	1.638	2.353	3.182	4.541
4	0.000	0.741	0.941	1.190	1.533	2.132	2.776	3.747
5	0.000	0.727	0.920	1.156	1.476	2.015	2.571	3.365
6	0.000	0.718	0.906	1.134	1.440	1.943	2.447	3.143

t-Test: Paired Two Sample for Means

	ICP-AES	*ICP-MS*
Mean	144.9	142.6333333
Variance	5976.3	5836.998851
Observations	30	30
Pearson Correlation	0.997045649	
Hypothesized Mean Difference	0	
df	29	
t Stat	2.077281509	
P(T<=t) one-tail	0.023369175	
t Critical one-tail	2.045229642	
P(T<=t) two-tail	0.04673835	
t Critical two-tail	2.363846073	

Using Excel for T-tests

- Use the Data Analysis Add-in Function and select the proper t-test for your analysis
  - Paired
  - Unpaired with equal variances
  - Paired with equal variances
- Or use Excel's insert function command