SEGH Society for Environmental Geochemistry and Health

BGS British Geological Survey

Quality Measurements for scientific writing outputs

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Context

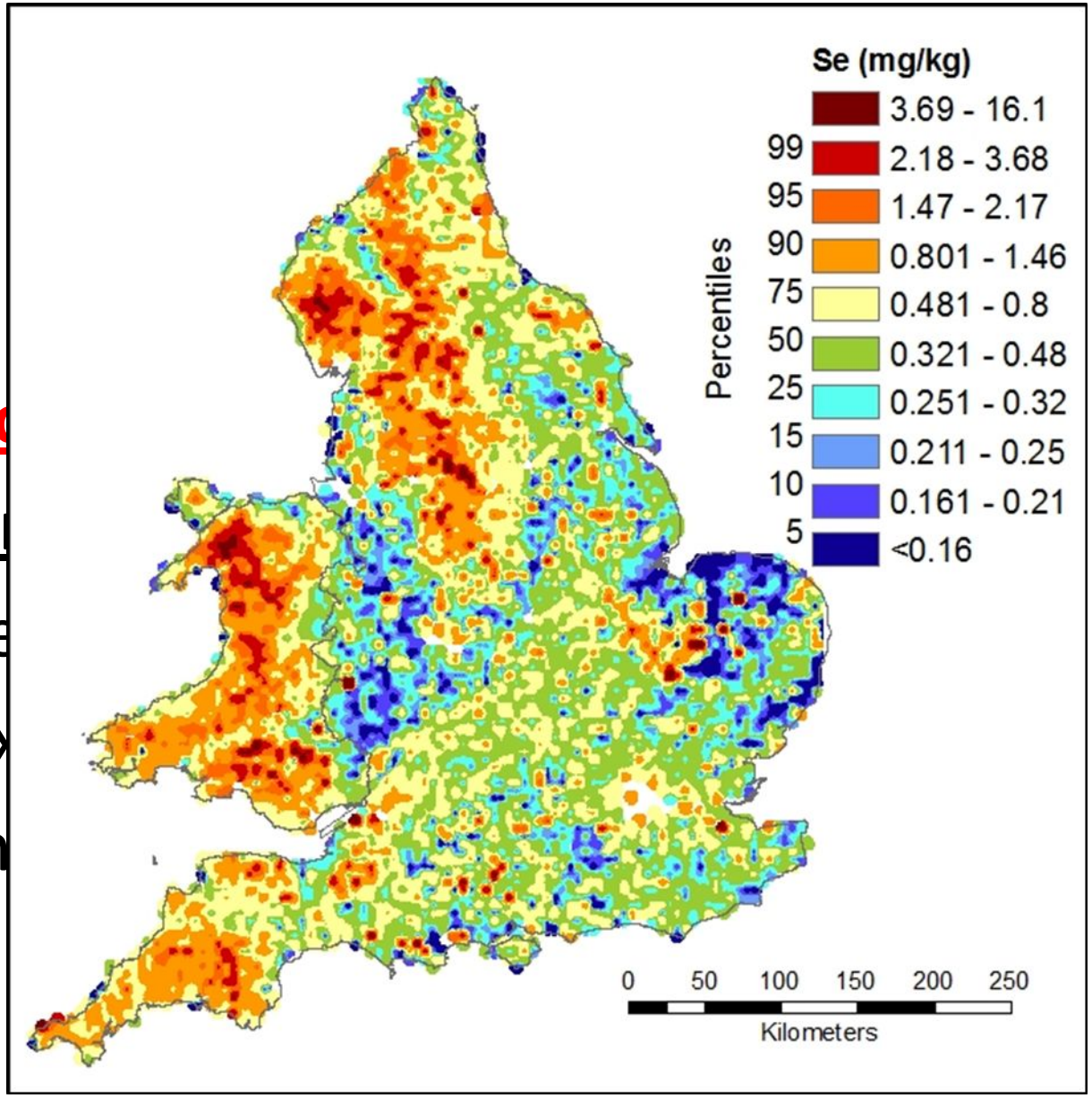
Many important decisions are based on the results of field or laboratory measurements.
Thus, it is important to have some indications on the quality of the results, i.e. client confidence/trust in your results to make a decision regulatory, commercial or scientific decision.

With globalisation and increasing competition for research funds, researchers are coming under increasing pressure:
(i) to **demonstrate the quality of their results** and
(ii) to **demonstrate their results can be compared to results obtained by other laboratories or for comparison with the scientific literature.**

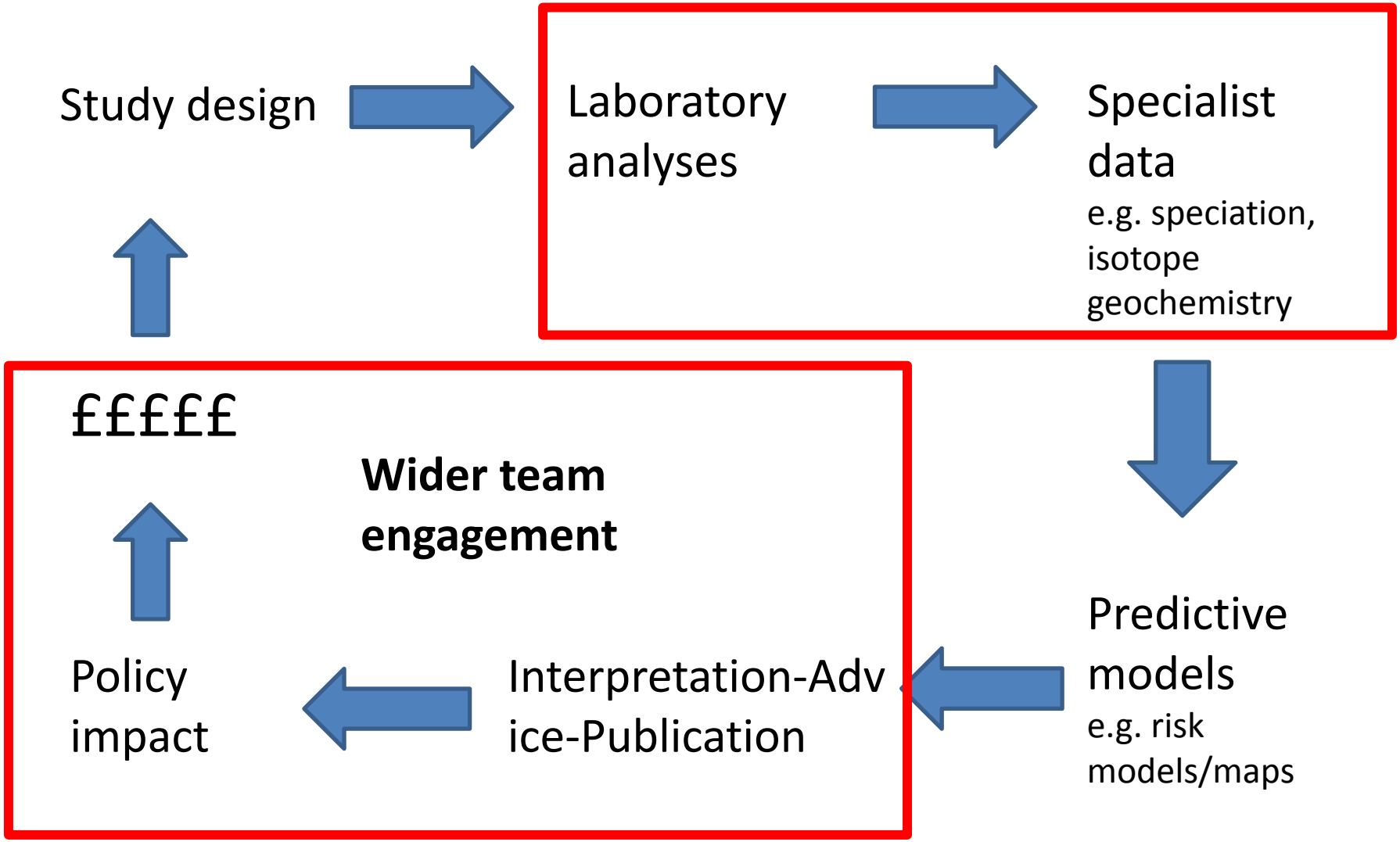
Everybody can measure, but not everybody can do professional quality measurements

Example applications for your data

- **Key co**
  - (1) **A**
  - (2) Te
  - (3) Ex
  - (4) In



Research cycle



Common problems in the literature

- Lack of or unclear Aim and objectives to achieve that Aim.
- Lack of or no detail for quality assurance measures – lack of confidence in measurements, field collection strategy etc.
- Therefore, questioning of complex statistics, graphical representation and interpretation.
- **Decisions founded on data could be costly without appropriate evidence for traceability.**
- There maybe legal or financial implications for your data without traceability and evidence for quality measurements

Food Security: inform agri-health policy

1. Hidden hunger
2. Influence of soil-type
3. Variation between food types
4. Household Survey
5. Alleviation strategies e.g. biofortification

<u>Why micronutrients? Health costs</u>

Iodine – IQ impaired by 10-15 points

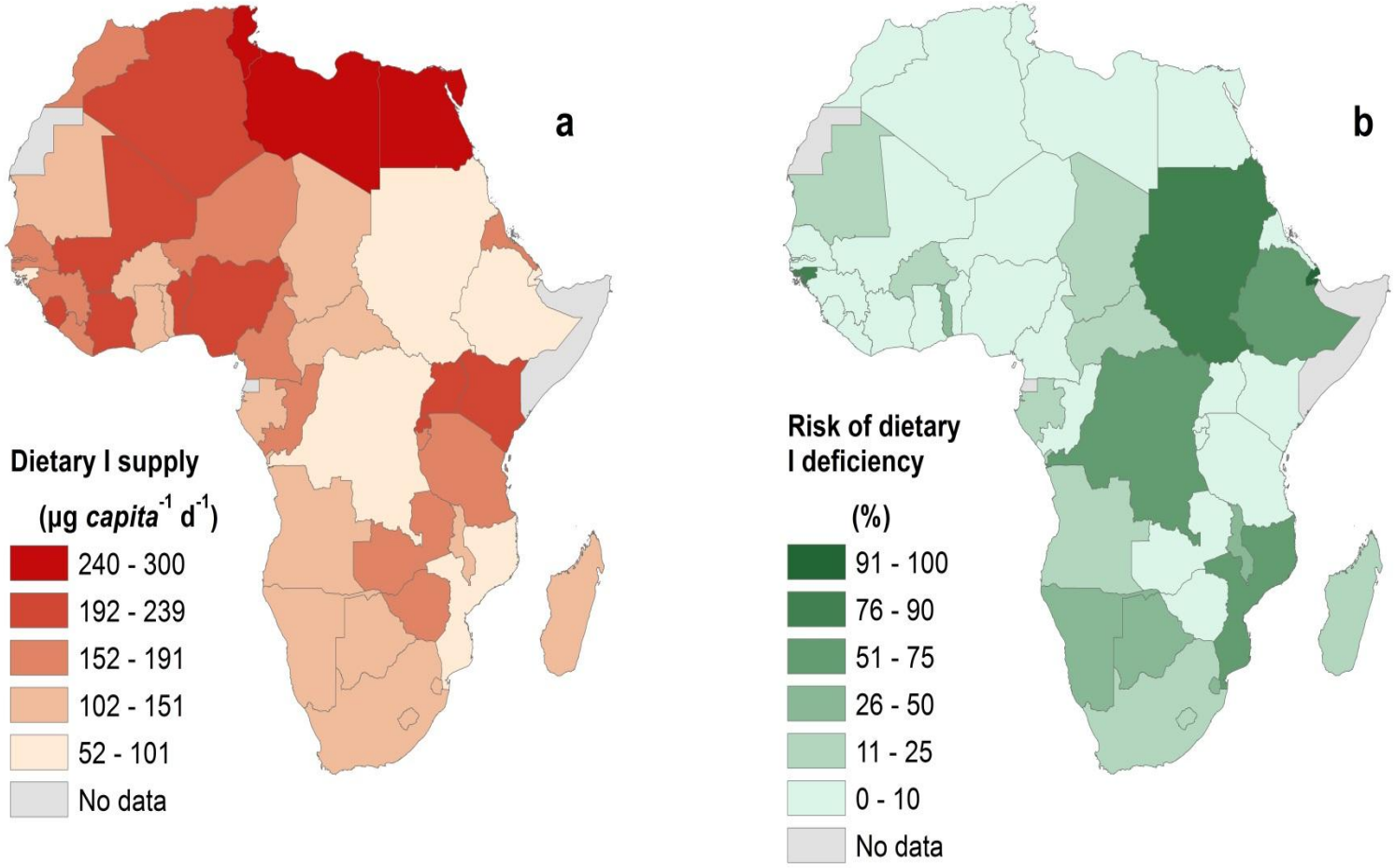
Iron – anaemia

Selenium – thyroid, immune function

Zinc – stunting, immunity

In Malawi ZnD ~ $51M per year using DALYs

Hidden hunger: High risks of Iodine deficiency in Africa



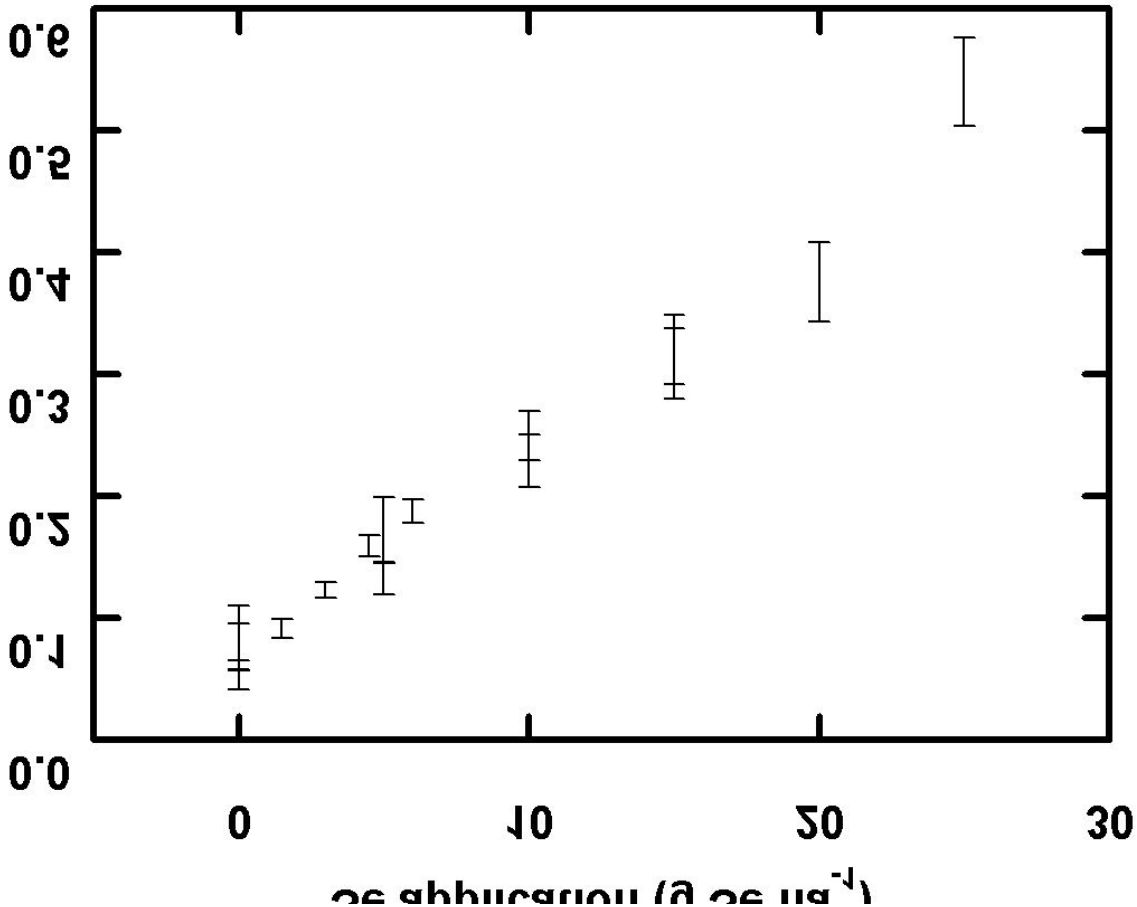
Joy et al. 2014. Dietary Mineral Supplies in Malawi, Physiologia Plantarum, 151, 208.

Alleviation strategies: Other

- Dietary diversification
- Crop breeding
- Food fortification
- Salt iodisation
- Supplements

Alleviation strategies: agronomy

Alleviation strategies: agronomy



Liquid drench $y = 0.019x + 0.061$

CAN+Se (granular) $y = 0.015x + 0.085$

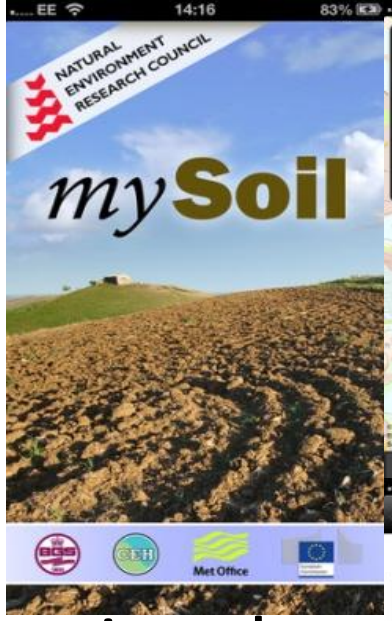
NPK+Se (granular) $y = 0.022x + 0.056$

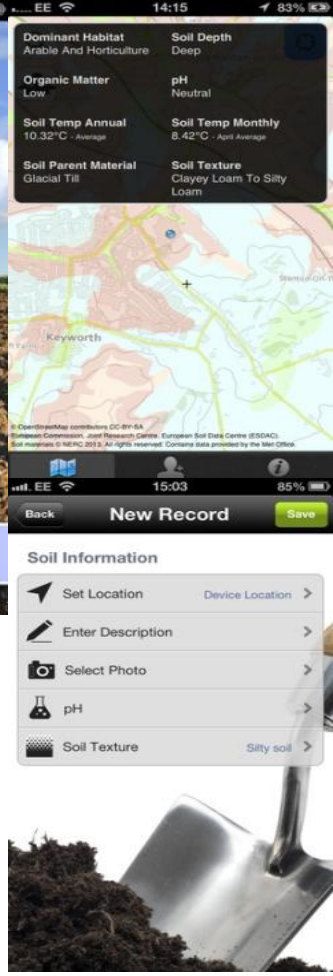
15-22 µg Se kg^{-1} grain . g^{-1} Se ha^{-1}

Chilimba et al., 2012

Gaps in Knowledge

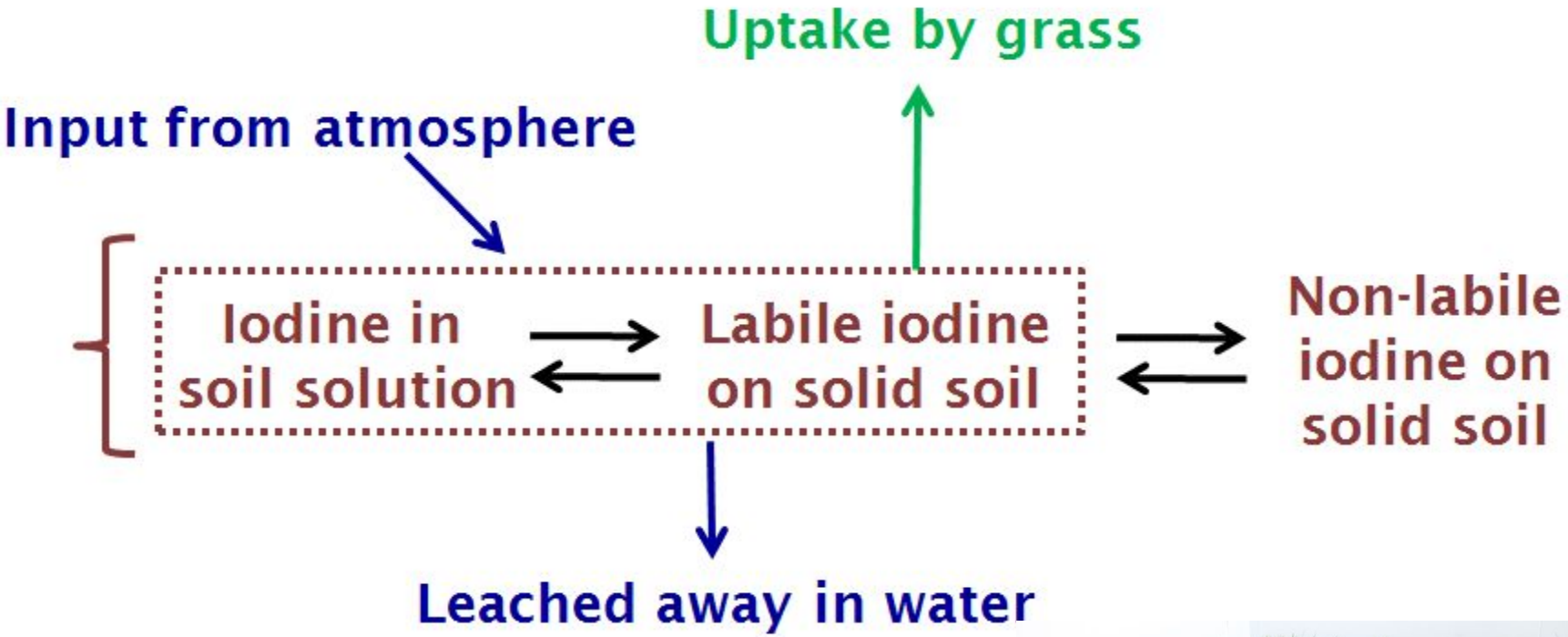
- Monitoring & storing data
- Communication

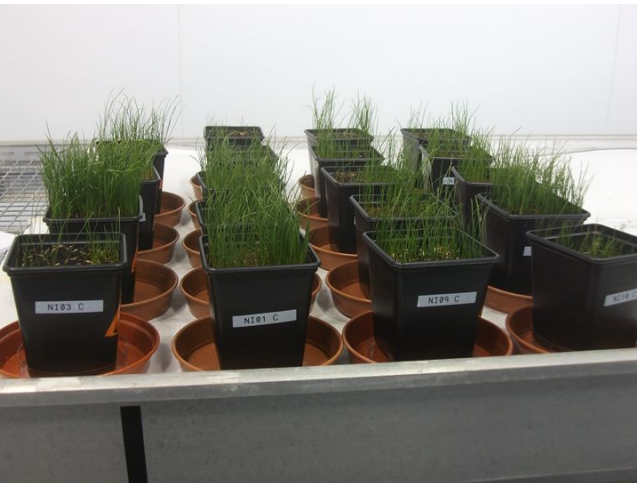




- Geospatial mapping, national & regional context – multiple data layers e.g. soil, health
- Targeted-evidenced intervention strategies
- Relevance for public policy
- <u>Such tools underpinned by measured data!</u>

Experimentation-Models





Predicting heavy metal solubility and speciation by WHAM-VII – Ed Tipping (CEH)

- The geochemical speciation model WHAM-VII will be used to predict Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, Cd, Pb and Se concentration in the solution phase of soil suspensions.
- Measured values of isotopically exchangeable metal (M_E) will be used as inputs to WHAM, representing the total reactive trace metal fraction in the soil suspensions.
- The modelled metal concentration in solution will be compared with measured values to assess the model performance.
- Speciation in solution and fractionation in the soil solid phase will be derived from the model output.

WHAM-IV Model inputs

Variable	Settings
Suspension condition	
Suspended particulate matter (SPM)	33.33 g L^{-1}
Temperature (K)	288.15 K (15°C)
PCO_2 (atm)	Measured bicarbonate concentration (DIC)
Soil pH Charge balance options	Measured in 0.01 M $Ca(NO_3)_2$ soil suspensions. No charge balance imposed i.e. a fixed (measured) pH value was used
Adsorption phase (g L^{-1})	
Clay content	MA soils: estimated from soil texture Urban soils: measured by laser granulometry
Fe, Al and Mn oxides	DCB extraction; converted to $Fe_2O_3.H_2O$, Al_2O_3 and MnO_2
Humic and fulvic acid	Measured by alkaline extraction
Colloidal fulvic acid	Estimated from measured DOC
Major cation and anion concentration (mol L^{-1})	
Dissolved major cations (Na, Mg, Al, K and Ca)	Concentration in filtered soil suspensions (0.01 M $Ca(NO_3)_2$) Precipitation option for Al: One mole of precipitated $Al(OH)_3$ forms 87 g of the binding phase within the particulate soil phase (S. Lofts., pers. comm.).
Fe^{3+} activity	Precipitation option for Fe: assumes that Fe^{3+} activity is controlled by $Fe(III)(OH)_3$ solubility, calculated within the model.
Dissolved nitrate (NO_3^-)	Solution concentration estimated as 0.02 M in the suspension
Total dissolved carbonate (all species)	Estimated from total inorganic carbon measured in solution
Trace reactive metal concentration in soil suspension (mol L^{-1})	
Total concentration Ni, Cu, Zn, Cd and Pb	Estimated from E-values (M_E)
Other settings	
Activity coefficient correction	Debye-Hückel
WHAM parameter data sets	Default master, solute and binding phase data bases.


F1598
F1598

Cornwall: private water supplies

- PHE concerned by perceived risk of arsenic in PWS – greater risk in Cornwall?

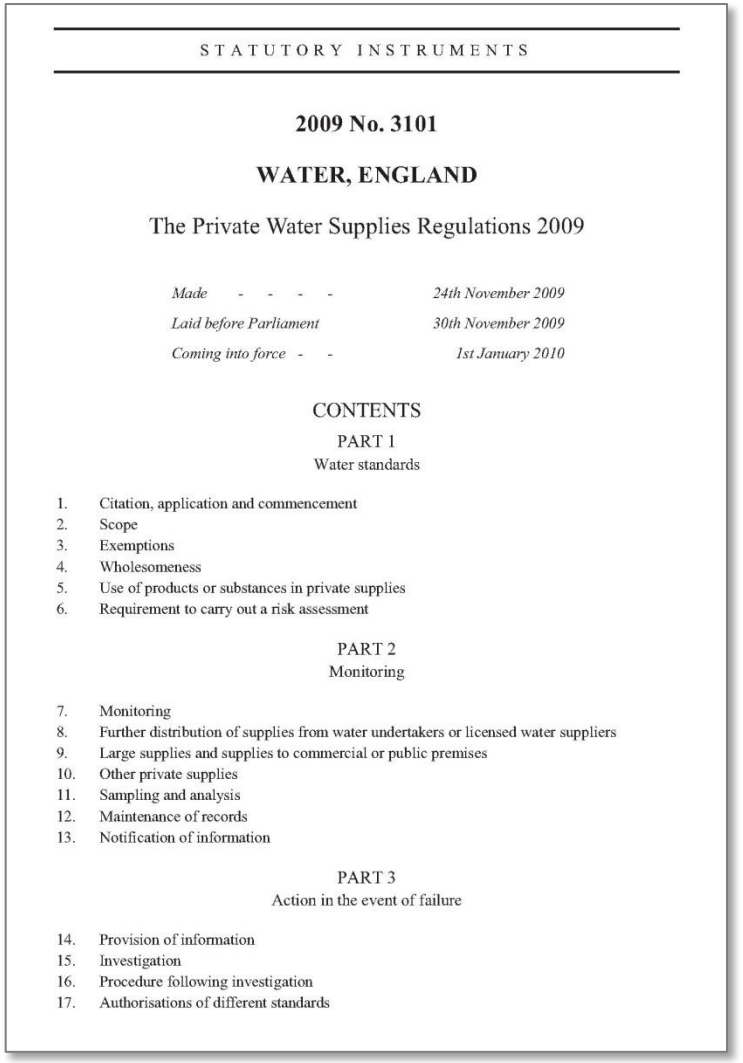
Cornwall: considerable numbers of private drinking water supplies.

- Paucity of information for inorganics related to water quality standards.

Drivers

- Health implications – Environment Public Health Tracking
- Model for predicting arsenic in PWS from geology?

- Biomonitoring phase



STATUTORY INSTRUMENTS

2009 No. 3101

WATER, ENGLAND

The Private Water Supplies Regulations 2009

Made - - - - *24th November 2009*
Laid before Parliament *30th November 2009*
Coming into force - - *1st January 2010*

CONTENTS

PART 1
Water standards

1. Citation, application and commencement
2. Scope
3. Exemptions
4. Wholesomeness
5. Use of products or substances in private supplies
6. Requirement to carry out a risk assessment

PART 2
Monitoring

7. Monitoring
8. Further distribution of supplies from water undertakers or licensed water suppliers
9. Large supplies and supplies to commercial or public premises
10. Other private supplies
11. Sampling and analysis
12. Maintenance of records
13. Notification of information

PART 3
Action in the event of failure

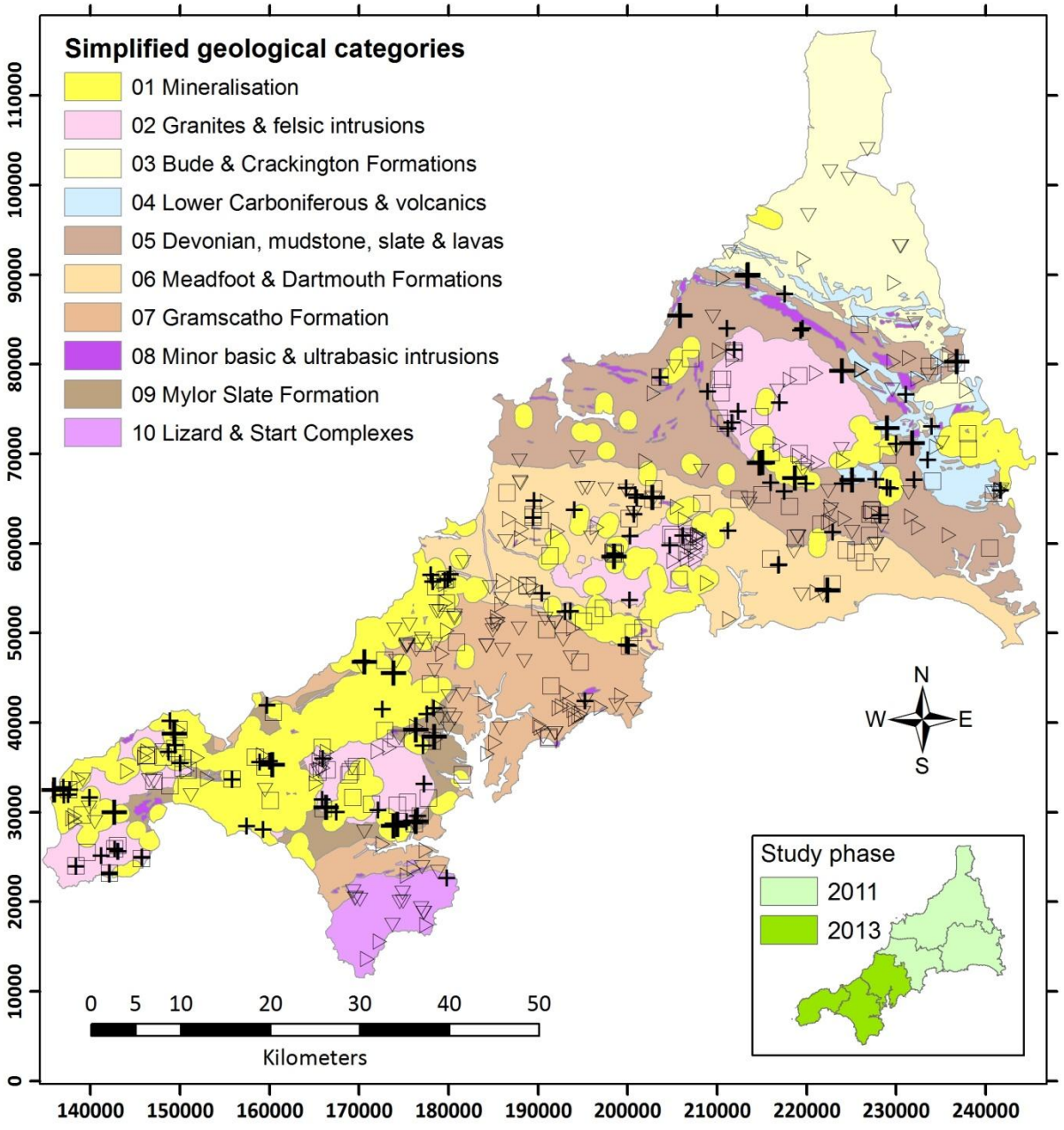
14. Provision of information
15. Investigation
16. Procedure following investigation
17. Authorisations of different standards

Sampling: *water collection at point of abstraction*

Groundwater samples were collected where this was (a) possible and (b) the schedule had sufficient time available.

Sampling not always possible prior to treatment and/or storage

Filtration of water for elemental analysis



The chemistry of private drinking water supplies in Cornwall

Concentration data for all drinking water samples

Arsenic (µg/L)

PCV	11 - 440
75th percentile	1.5 - 10
50th percentile	0.38 - 1.4
25th percentile	0.16 - 0.37
	<0.15

Parameter	Arsenic (As)
Prescribed concentration or value (PCV) - maximum concentration	10 µg/L
Total number of samples	491
Samples above the PCV	27
Percentage of samples above the PCV	5

Analysis by ICP-MS.
Map compiled June 2013.

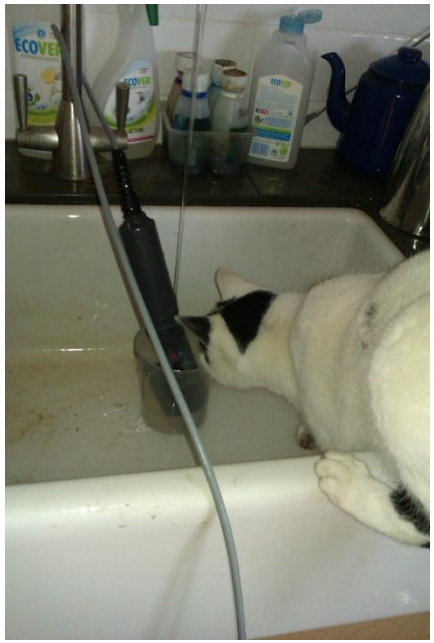
British Geological Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL

Public Health England

Soil/dust ingestion

Wind-blown soil and dust

Private Water Supplies



Diet

Quality measurements

- Geochemistry crosses boundaries
- Nexus of **environmental-resource security-ecosystem-health** studies.

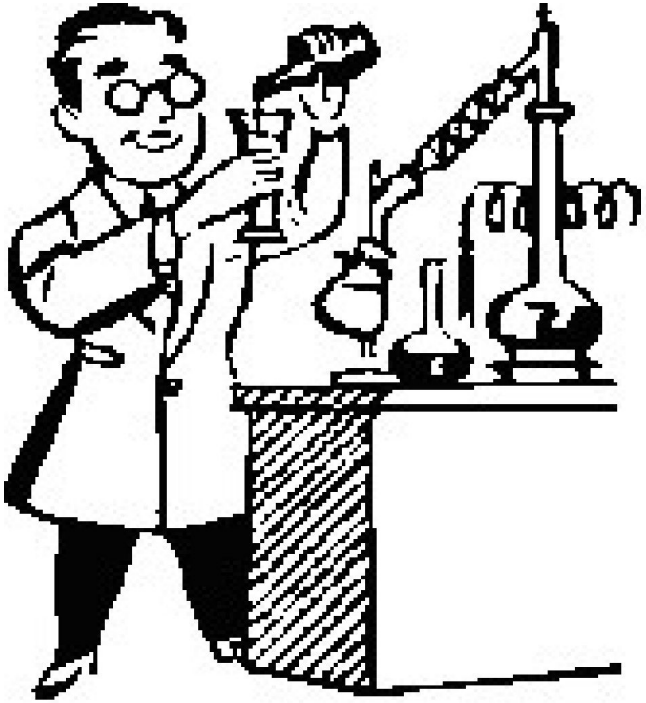
- Make sure you know how your data was produced

- Do you have confidence in the data-evidence?

- Would you be comfortable being questioned on the validity of your data?

- It can feel very personal – plan quality measurements into your sampling strategy

- Remember the Aim of the study and the objectives to achieve that Aim.



What should you know?

- It does not have to be expensive.

Quality Management

- You do not need accreditation for good quality management – accreditation is expensive to set-up and to maintain.
- However, the principles can be applied anywhere.
- Not funding dependent – a Quality Assurance system requires lab staff and management to take responsibility and support the process.
- Where resources are limited, networks can assist – peer review.

International Standards for Quality Management

- ISO 9001:2015 – generic management Standard
  - refers to an organization's structure for managing its activities
  - can be applied to any business enterprise, public administration, or government department
- ISO 17025:2005 – technical competency Standard
  - for laboratories - specifying the additional requirements for demonstrating technical competence
- ISO 17025:2017 –released 2019
  - based on ISO 9001:2015
  - specifies the additional technical requirements

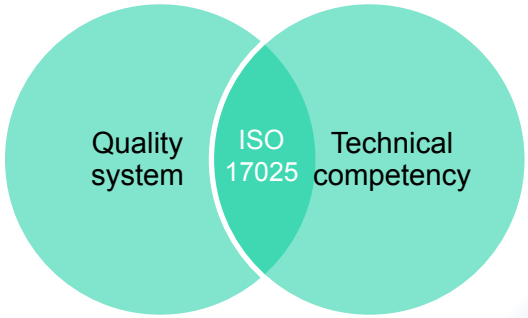
ISO/IEC 17025:2005

4. Management requirements

4.1. Organization
4.2. Management system
4.3. Document control
4.4. Review of requests, tenders, contracts
4.5. Subcontracting of tests
4.6. Purchasing services and supplies
4.7. Service to the customer
4.8. Complaints
4.9. Control of non-conforming work
4.10. Improvement
4.11. Corrective actions
4.12. Preventive actions
4.13. Control of quality records
4.14. Internal audits
4.15. Management review

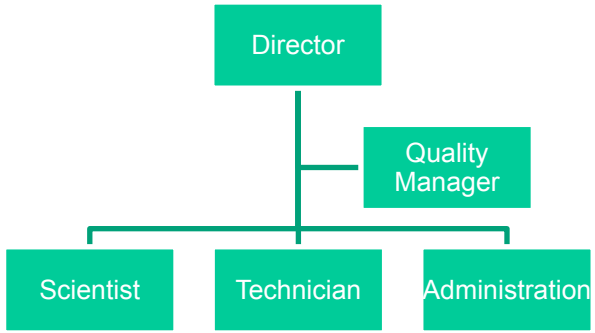
5. Technical requirements

5.1. General
5.2. Personnel
5.3. Accommodation & environmental conditions
5.4. Test methods and validation
5.5. Equipment
5.6. Measurement traceability
5.7. Sampling
5.8. Handling of Test items
5.9. Assuring the quality of test results
5.10. Reporting the results



Management Requirements

Organization



- The organization will be held legally responsible
- Work carried out at permanent or mobile facilities
- Define responsibilities of key staff - conflict of interest
- Staff to have authority, responsibility and resources
- Ensure protection of confidential information
- Define structure and specify interrelationships
- Quality Manager with direct access to ~~top~~ management
- Ensure staff are aware of the relevance of their roles
- Effective communication processes

Management system

- Establish, implement and maintain documentation of policies and procedures - review
- Management commitment to stated standard of service and to improve
- Staff to familiarize themselves with and implement the policy
- Define roles al Management

Document control

- Establish procedures for review and approval
- Approval and issue
  - Availability at point of use
  - Periodic review
  - Version control (archiving)
  - Unique identification
- Change review and approval
  - Traceability
  - Hand written or computerized

Service to the customer

- Cooperate to clarify request
  - Access to witness
- Confidentiality
- Communication
  - throughout the work
- Seek feedback
  - Analyse for improvement

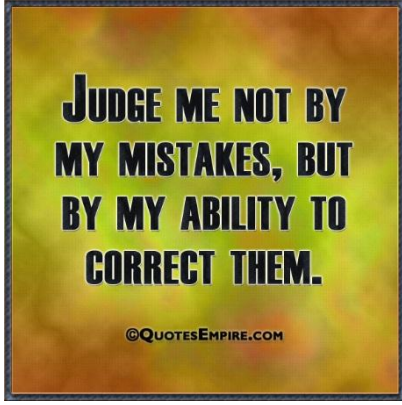
Complaints

- Policy and procedure for handling complaints
- Keep records of complaints, investigations and actions

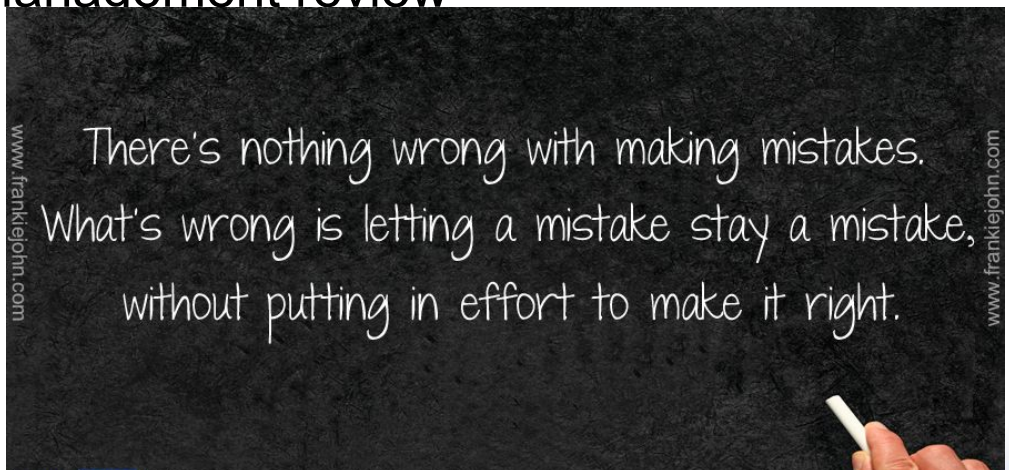
Control of non-conforming work

- Policy and procedure for investigation when any aspect does not conform
  - Results of Audits or other observations
  - QC failures
- Responsibility for who does what
- Evaluation
- Corrective and Preventative Actions
- Notification or recall?
- Authorize resumption

Corrective actions



- Continually improve the effectiveness of the management system
  - Quality policy and objectives
  - Audit results
  - Corrective and Preventative Actions
  - Management review



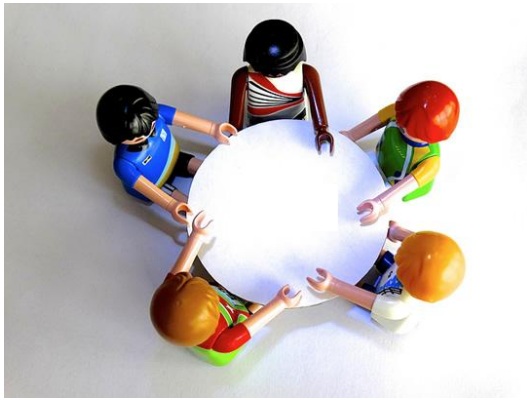
Control of quality records

- Identification, collection, indexing, access, filing, storage, maintenance and disposal
- Readily retrievable suitable environment
- Secure and in confidence
- Protect and back up electronic records

Internal audits

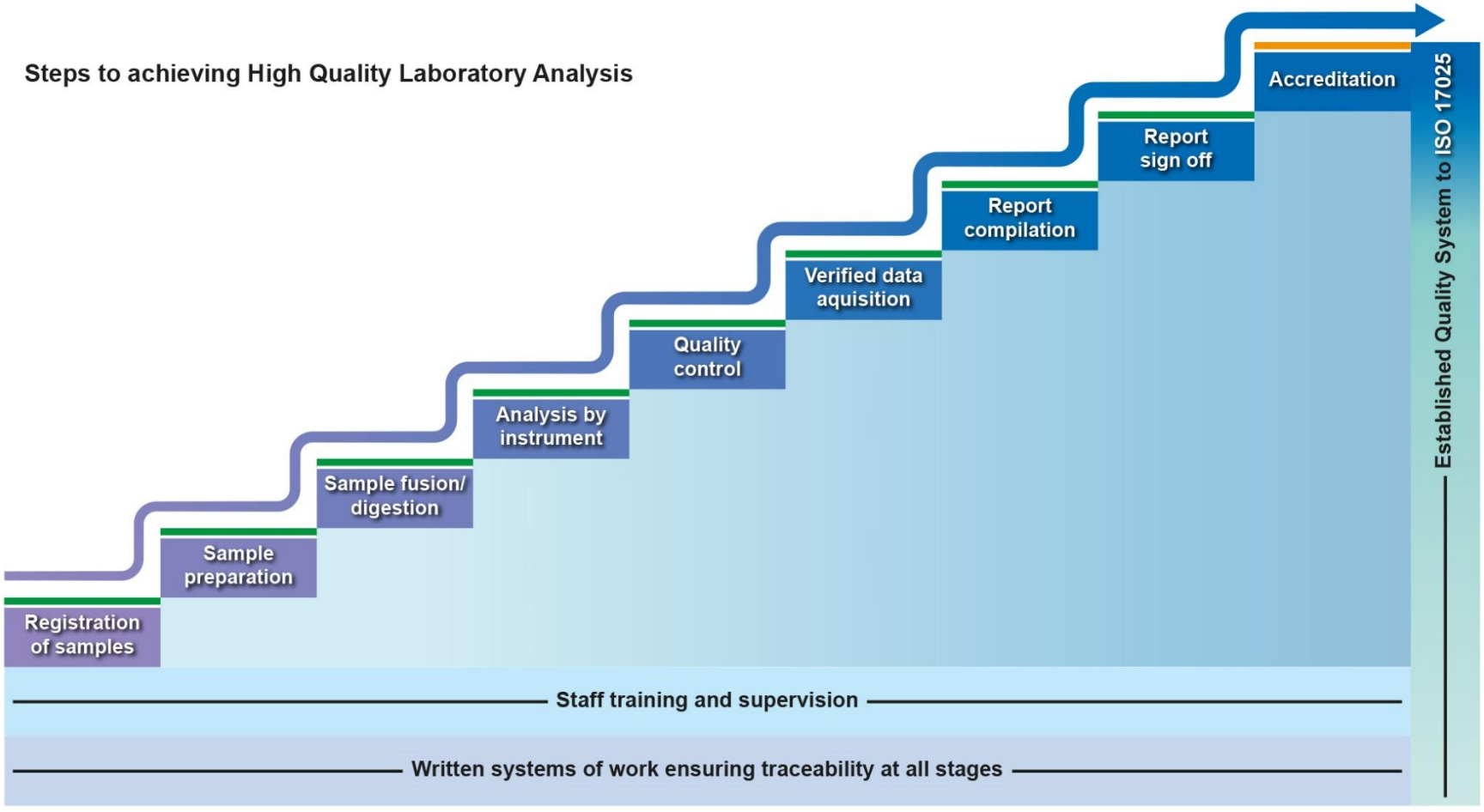
- Predetermined schedule and procedure
- Verify operations continue to comply
- Address all elements of Standard
- Carried out by trained and qualified personnel
  - Independent of activity
- Timely response
- Notify clients if results have been affected
- Implementation and effectiveness of Corrective Actions

Management review



- Review of management system and testing ~~by top management~~
  - Suitability
  - Internal and external audits
  - Corrective and Preventative Actions
  - Interlaboratory comparisons and Quality Control
  - Changes in work load
  - Customer feedback
- Recommendations for improvement
- Actions carried out in a timely manner

Technical requirements



Personnel

- Competence – operation, evaluation, reporting
- Qualification – training, education, experience
- Training goals and training needs
- Employed – supervised and competent
- Job descriptions for key staff
- Authorization
  - Training records

Accommodation and environmental conditions

- Ensure environmental conditions do not invalidate
- Monitor and control:

  sterility, dust, electromagnetics, radiation, humidity, electricity, lighting, temperature, sound, vibration, etc.
- Effective separation for incompatibles
- Laboratory access
- Housekeeping

Test methods and validation 1

- Select appropriate methods – inform client
  - Client preference – define, suitability
- Plan a method for – revise
- Qualified operator
- Non-standard methods by agreement
- Document

Method description - SOPs

- Appropriate identification and specified scope
- Parameters and ranges
- Equipment (performance requirements)
- Reference standards and reference materials
- Environmental conditions - stabilization
- Labelling, checks on samples, instrument checks, how to record results, safety measures
- Approval criteria
- Recording and presenting of data
- Uncertainty

Test methods and validation 2

- Validation
  - Confirmation by examination
  - Provision of objective evidence
  - Range and accuracy…
- Estimate uncertainty of measurement
  - identify components – performance, scope, experience
- Control of data – making checks
  - document computer programs

Method performance

- Sampling, handling and transportation
- Calibration using traceable standards
- Comparison of data with other methods/results
- Interlaboratory comparisons – PT schemes
- Systematic assessment of factors influencing results
- Theoretical understanding and practical experience - Uc

range accuracy detection limit
selectivity linearity repeatability
reproducibility robustnessmatrix sensitivity

Equipment

- Furnish with all required items for work
- Capable of required accuracy before use
- Checked and calibrated
  - Identify calibration status/out of use
- Use by authorized personnel
- Operating and maintenance instructions readily available
- Equipment records and unique identification
- Safe handling, storage, use and ce

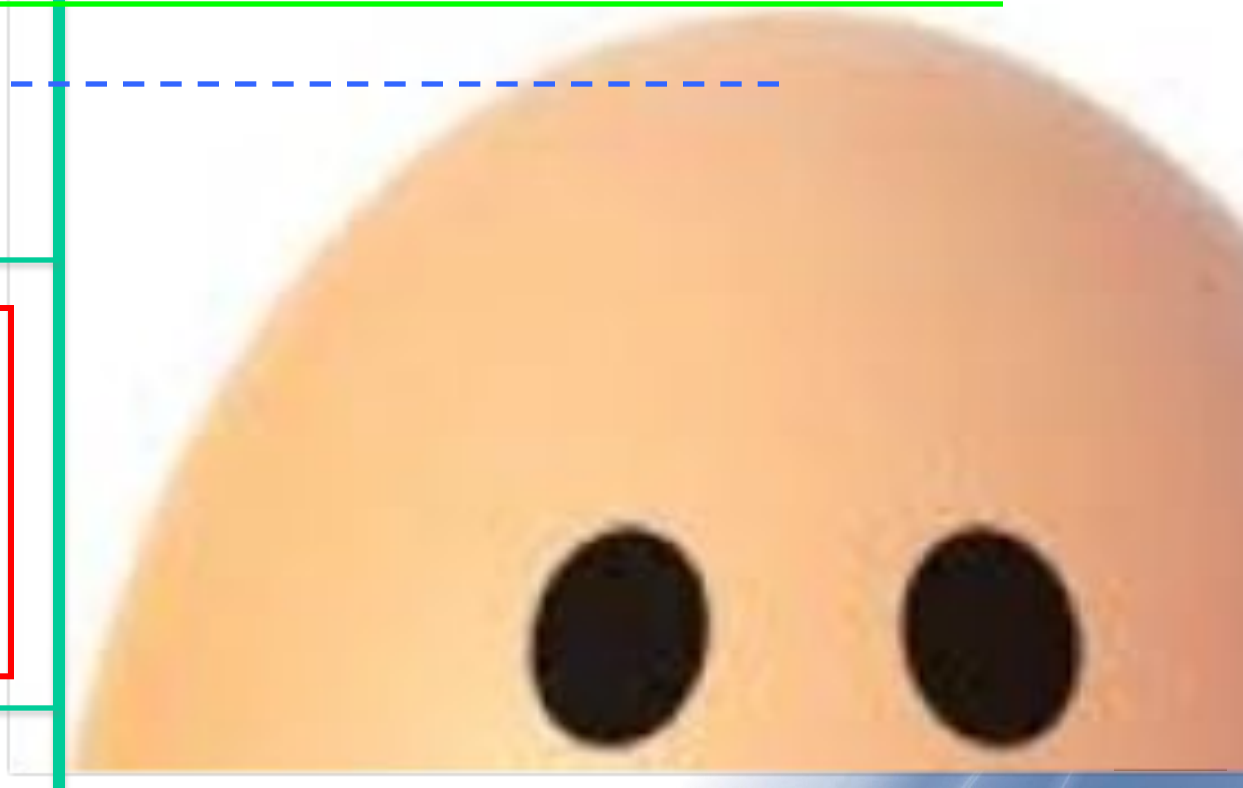
Everybody can measure, but not everybody can do professional quality measures.

for one egg, one ruler,

but different people==> different measures.

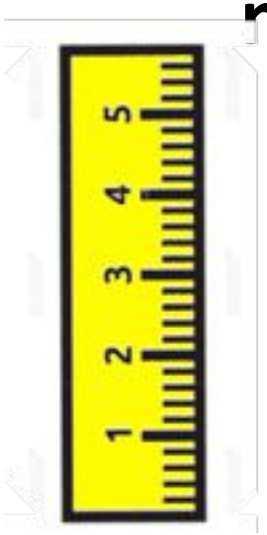
cannot know error

cannot know ‘true value’



can only minimise the errors…

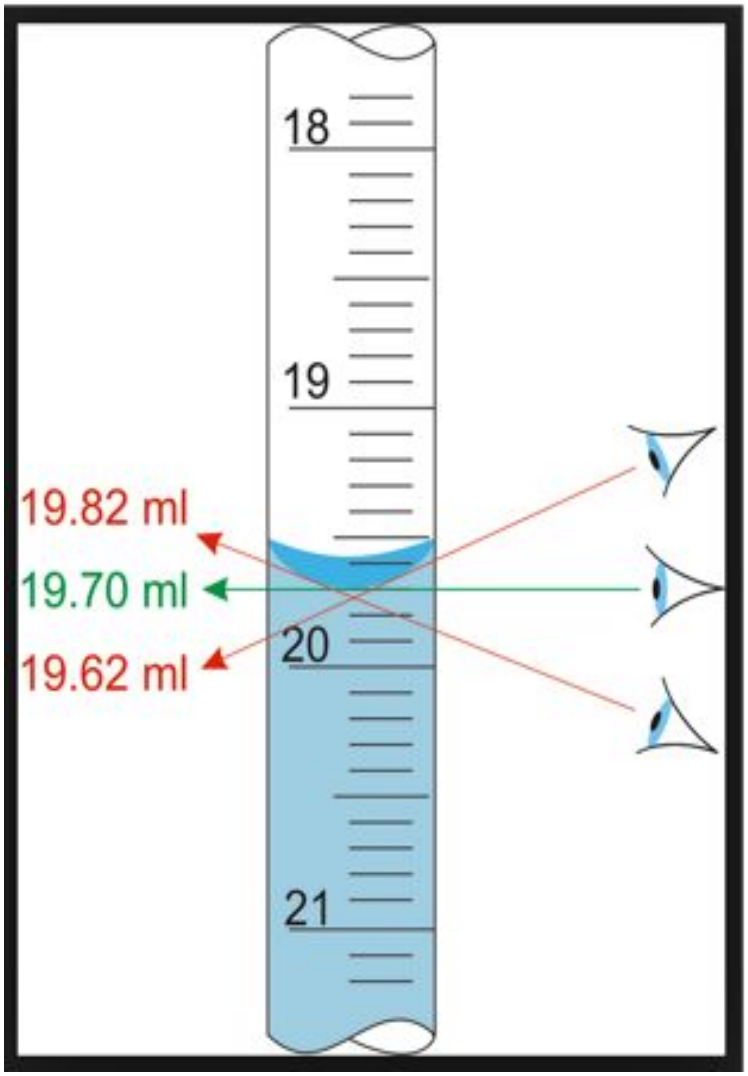
measure the egg….

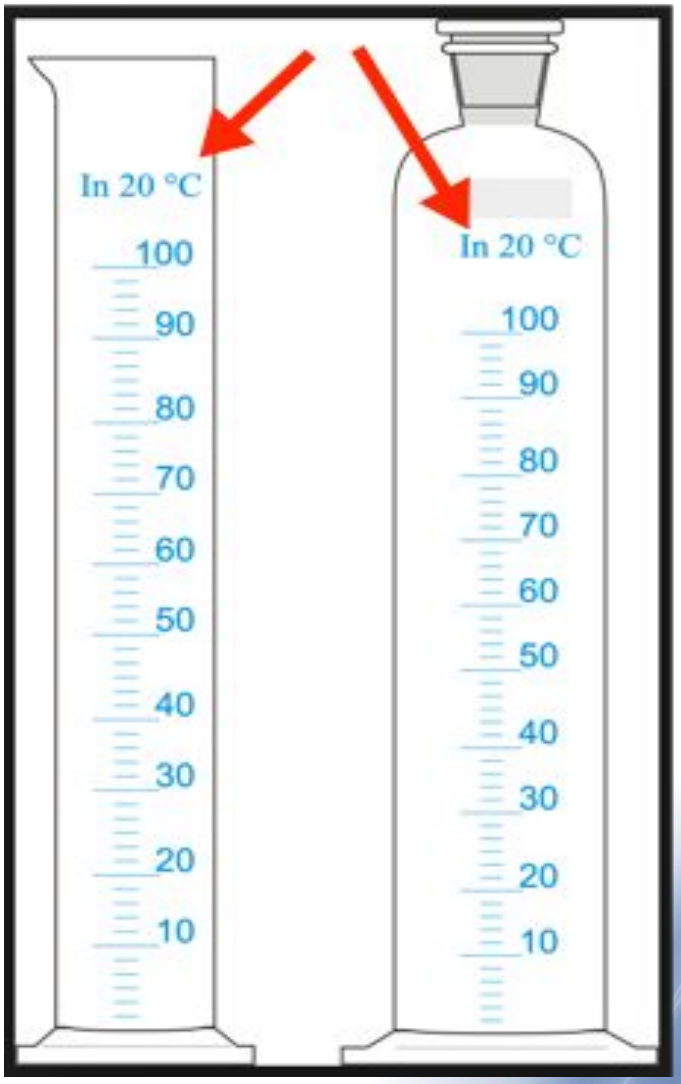


METROLOGY teach us that
all measures contain errors - UNCERTAINTY:

measure = true value +/- error

Factors e.g. operator / environment



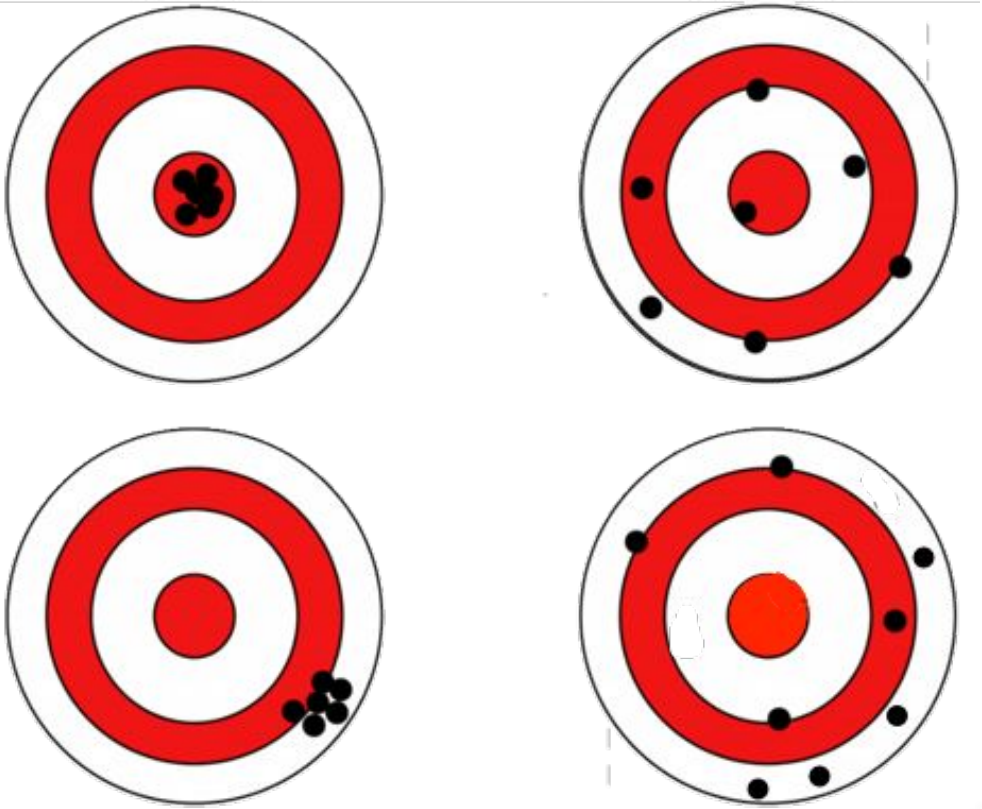


Precision: high low

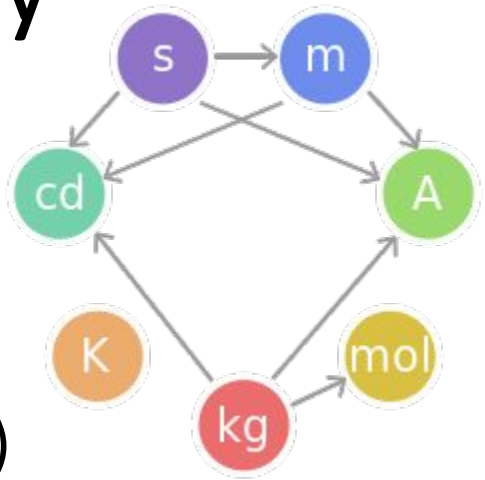
Accuracy:

high

low



Measurement of traceability

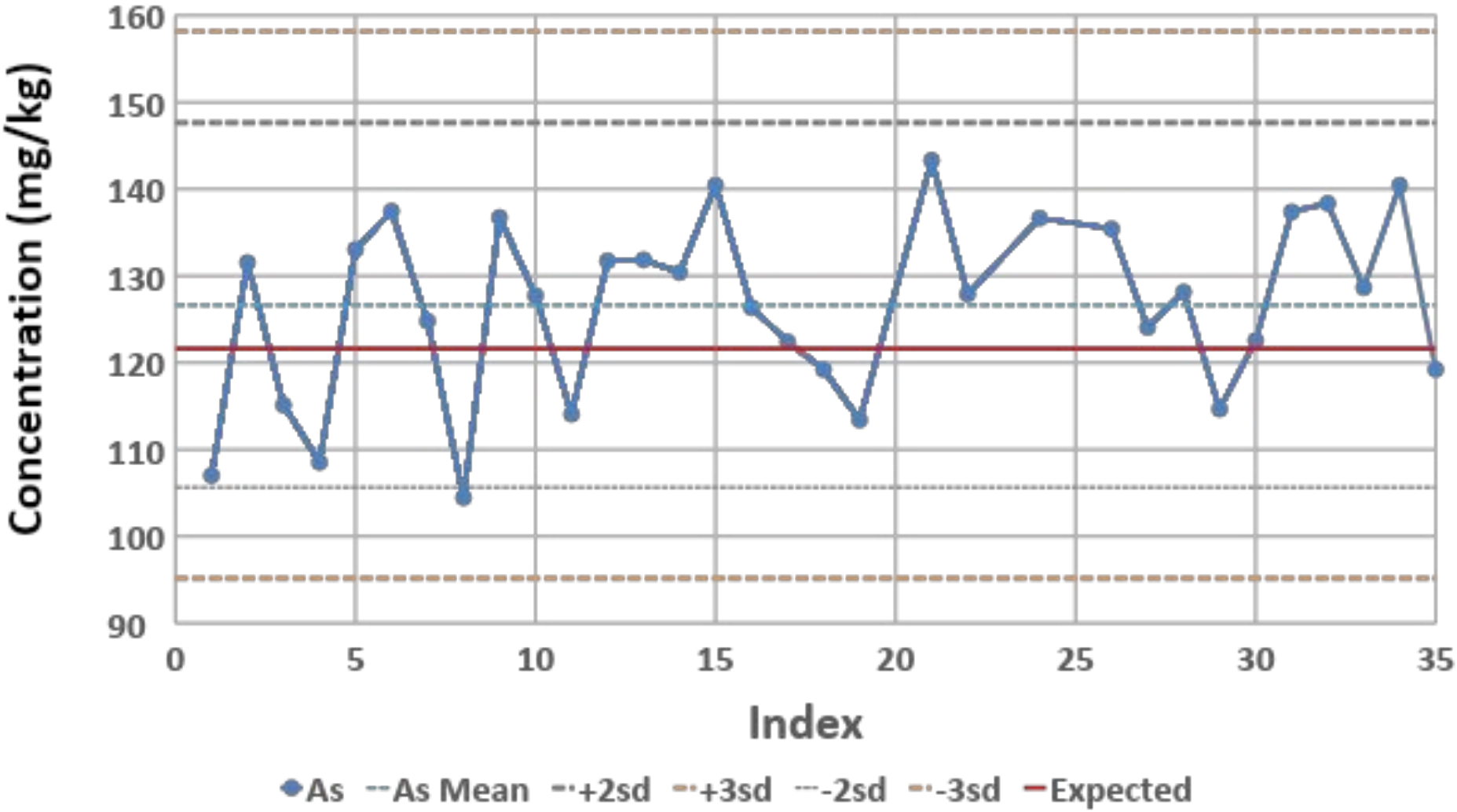


- Calibrate all equipment before use
  - following set procedure
- Traceable to International System of Units (SI)
  - reference to a primary standard
- Calibration standards
- Certified Reference Materials (CRM)
- Intermediate checks to maintain confidence in the calibration
- Handling, storage - prevent contamination/deterioration

Assuring the quality of test results

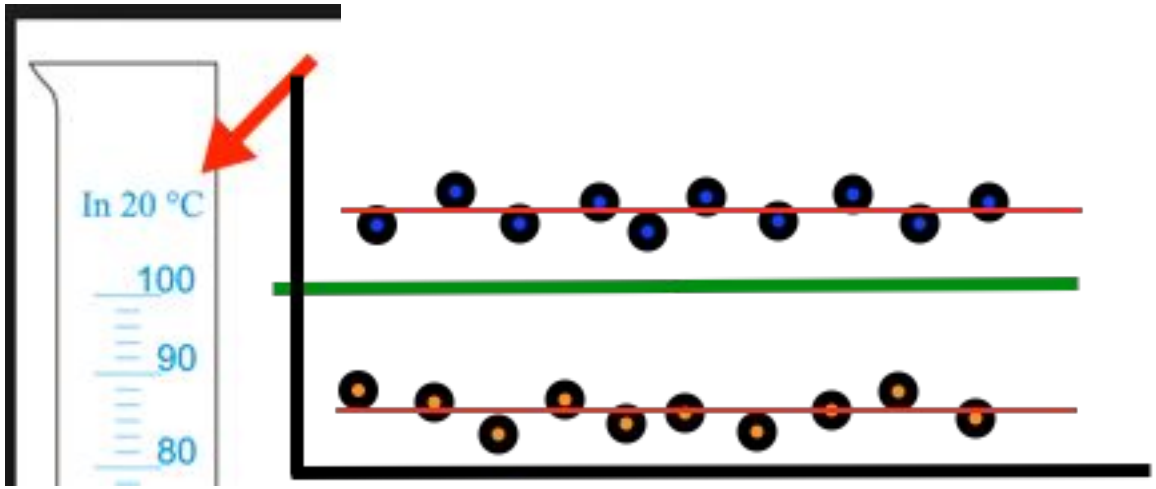
- Quality Control (QC) procedures
- Record results - to view trends
- Statistical evaluation of QC data
- Plan and review monitoring of QC data
  - CRMs, secondary standards
  - Proficiency Testing schemes - EPTIS
  - Replicates and repeats
- Predefined acceptance criteria
  - Shewhart chart – Westgard rules
- Planned action to correct and prevent

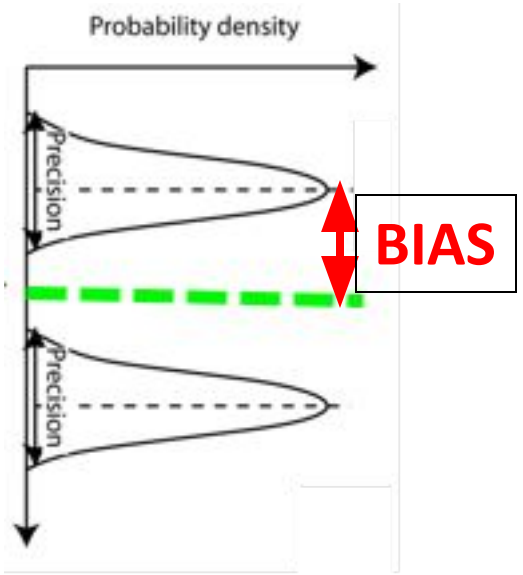
Shewhart QC chart



Analytical errors can be of 2 categories:

2. **Systematic** or ‘predictable’, regular deviation from the "true" value.





Quality management principles

Customer focus – meet customer requirements and expectations

Leadership – to establish unity of purpose and direction

Engagement of people – competent, empowered staff enhance capability

Process approach – a coherent system achieves consistent and predictable results

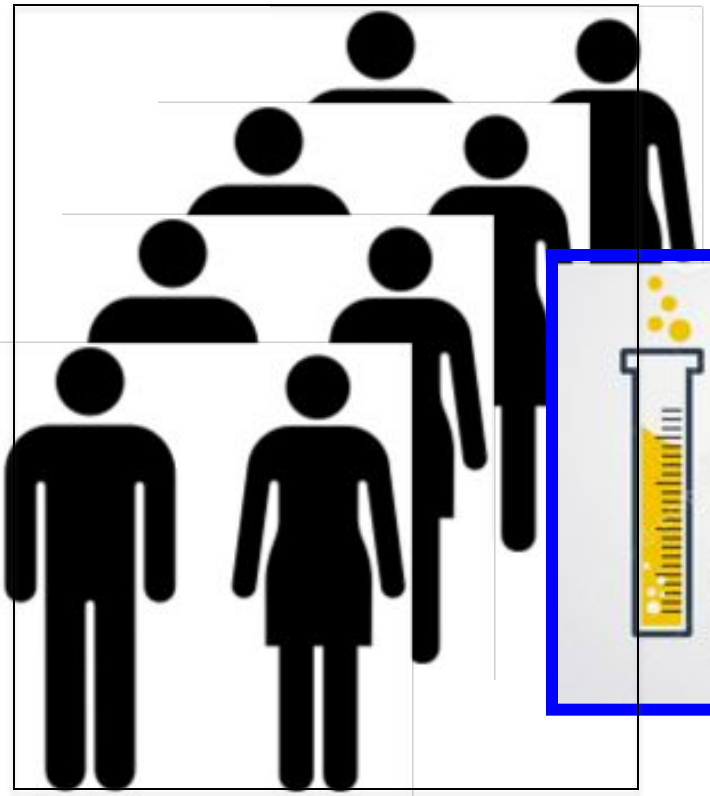
Improvement – leads to successful organisations

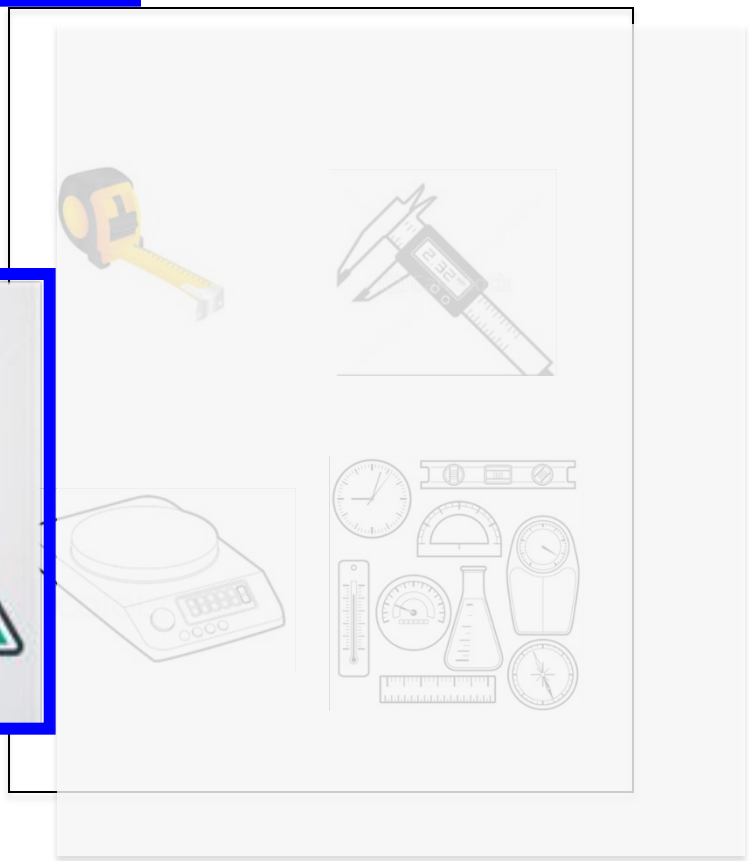
Evidence-based decision making - produce desired results.

Relationship management – for sustained success

ANALYSIS:

People **+ chemical reactions +** **Instruments**





Staff but also… students

every body must work the same way…. how? SOP !

Quality Management-summary

- Documented SOPs, clearly defined responsibilities and checks on data

  → promote reproducibility

  → promote safe working practices

  → provide confidence in data outputs

Traceability from arrival of sample to reporting of data

Evaluate and monitor – do not ignore erroneous data!

What can you do?

- Networks exist to facilitate quality management e.g. GLOSOLAN
- Reference Materials could be made in-house
- Inter-laboratory comparisons could be with colleagues at other local institutions or even ask a lab with a quality management system help your lab
- Take part in Proficiency Testing schemes – particularly when they are free! (Glosolan) - **Every lab can improve**.
- Devise a plan to remedy data problems – DO NOT IGNORE- ask for help.
- Hopefully we will see better confidence in measured data in the literature and potential for income generation kept within developing countries
- Resources kept in-country with improved confidence in data for Applied Geochemistry

Seek help - network

- Royal Society of Chemistry (RSC) – travel grants, secondments (ACTF), plus lots of material on www.rsc.org
- Society for Environmental Geochemistry and Health www.segh.net

- FAO-UN Global Soil Laboratory network (GLOSOLAN) – harmonisation of procedures worldwide – Head of Afrilab section – Joseph Uponi (Nigeria)