Consolidate multiparameter wet chemical testing to speed up your laboratory research with discrete analysis technology

Tuesday, March 28, 2023

Sean McCormick - Manager, Application Scientists, IC/SP/DIA
Gary He - Product Marketing Manager, Gallery Discrete Analyzers

ACS Spring 2023 Thermo Fisher Scientific sponsored session

The world leader in serving science

Agenda

1. Broad application range with discrete analyzers
2. Consolidate multiparameter testing with discrete analyzers
3. Testing technique comparisons
4. Real world use experiences

Over 20 years of experience with discrete analyzers

New model for water testing applications

2000's

Konelab

Aquakem

2010's

Gallery, Gallery Plus, Beermaster

2021

Enzyme Master

2023

Aqua Master

Global network of experienced remote and field-based service engineers and application specialists

Continuing to deliver state-of-the-art discrete analyzers to address customer needs

Broad range of applications for Thermo Scientific™ Gallery™ discrete analyzers

Environmental

- Drinking water
- Wastewater
- Soil

Food

- Agriculture
  - Soil
  - Plant extract
  - Fertilizer
- Grain research
- Dairy
- Food additives
- Potato chips
- Honey

Industrial

- Raw water
- Process water
  - Produced water
  - Crude desalting
  - Hydraulic fracking
  - Cooling water
- Wastewater
- Fermentation metabolites

Beverage

- Wine
- Beer, cider
- Fruit juices
- Yogurt drinks

Enzyme

- Enzyme manufacturers
- Detergents
- Biofuels
- Animal feed
- Oligonucleotide

Parameters applicable to Gallery systems

Food and beverage applications

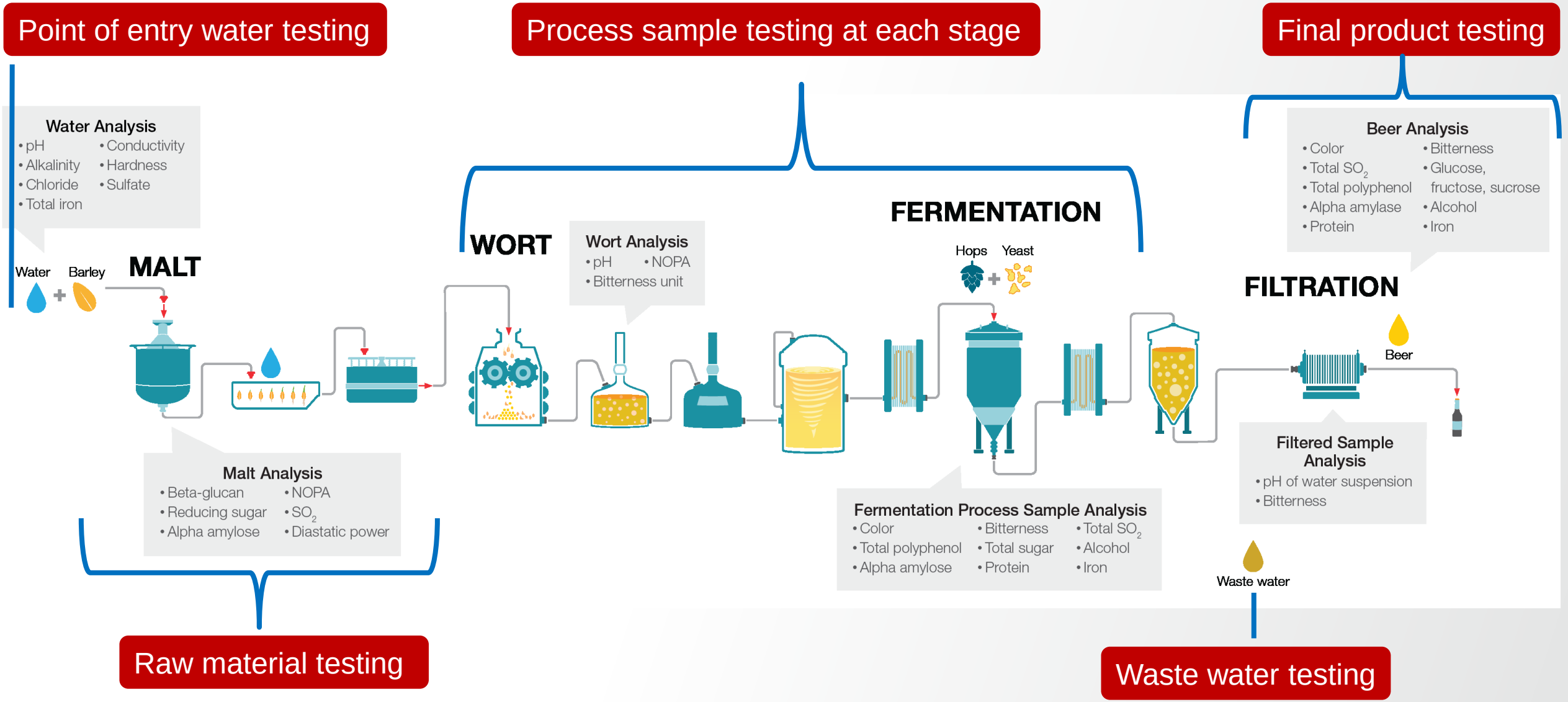
Organic acids	Feed water and waste water	Process critical parameters
Acetic acid Ascorbic acid Aspartic acid ß-Hydroxybuturic acid Citric acid Color D-Gluconic acid D-Isocitric acid D-Lactic acid D-Malic acid Formic acid* Gluconic acid Glycolic acid L-Ascorbic acid L-Lactic acid L-Glutamic acid L-Malic acid Oxalic acid pH Succinic acid Tartaric acid	Free and total cyanide* Iron Nitrate Nitrite Phosphate pH and conductivity Total Kjedahl Nitrogen (TKN)* Total Oxidizable Nitrogen (TON) Total phenol* Total phosphate* Alkalinity* Total Hardness Chloride Sulfate	Acetaldehyde Alcohol by volume (low) Alpha-Amino Nitrogen (NOPA) Alpha amylase Beta glucan Bitterness* Cholesterol Ethanol Glutamate Glycerol Hesperidin Hydroxymethylfurfural Hydroxyproline L-Asparagine Total polyphenol* Total protein Urea
Titration	**Cations**	**Sugars**
Free and total SO_2 Total acidity*	Ammonia Calcium Copper* Magnesium Potassium	D-Fructose D-Glucose D-Mannitol* D-Sorbitol / Xylitol* Lactose* Sucrose

Drinking water, industrial water, and waste water applications

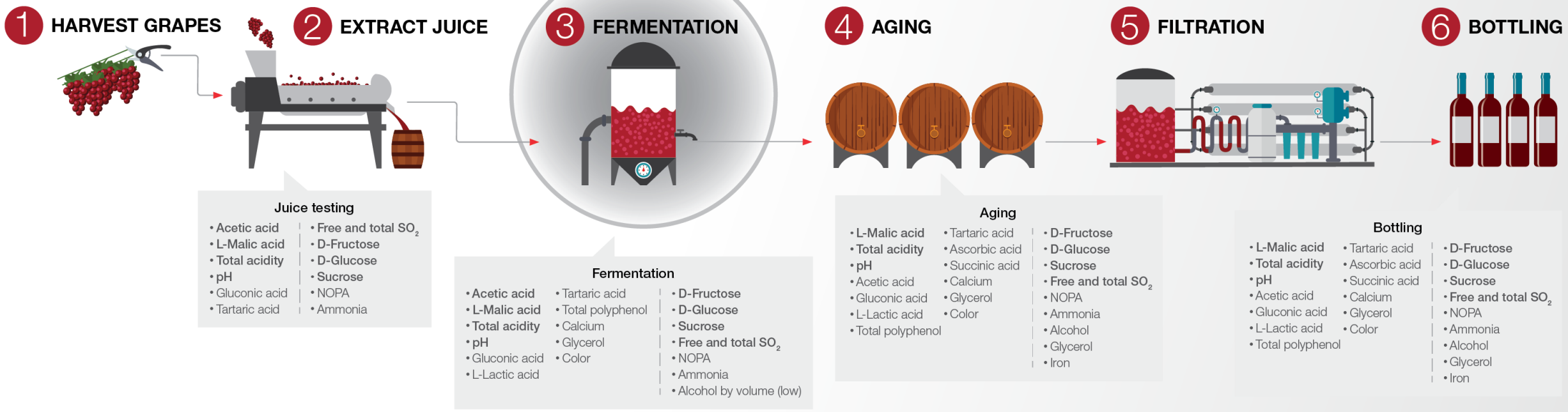
Anions	Corrosion inhibitors	Cations and metals	Basic water analysis
Bromide Chloride Fluoride Nitrite Nitrate Sulfide* Sulfate Sulfite Thiosulfate*	Ammonia Molybdenum Nitrite Phosphate Zinc	Aluminum* Ammonia Boron* Copper* Hexavalent chromium Manganese* Molybdenum Total iron Zinc	Alkalinity* COD Total hardness
Environmental	**Scaling**	**Nutrients**	**Measurements**
Aluminum* Boron* Free and total cyanide* Manganese* Total Kjeldal Nitrogen (TKN)* Total phosphorus Total phenol* Total Oxidizable Nitrogen (TON) Sulfide Urea	Calcium Magnesium Silica	Ammonia Nitrite Nitrate TKN TON Total phosphorous	pH and conductivity

*Third party reagents.

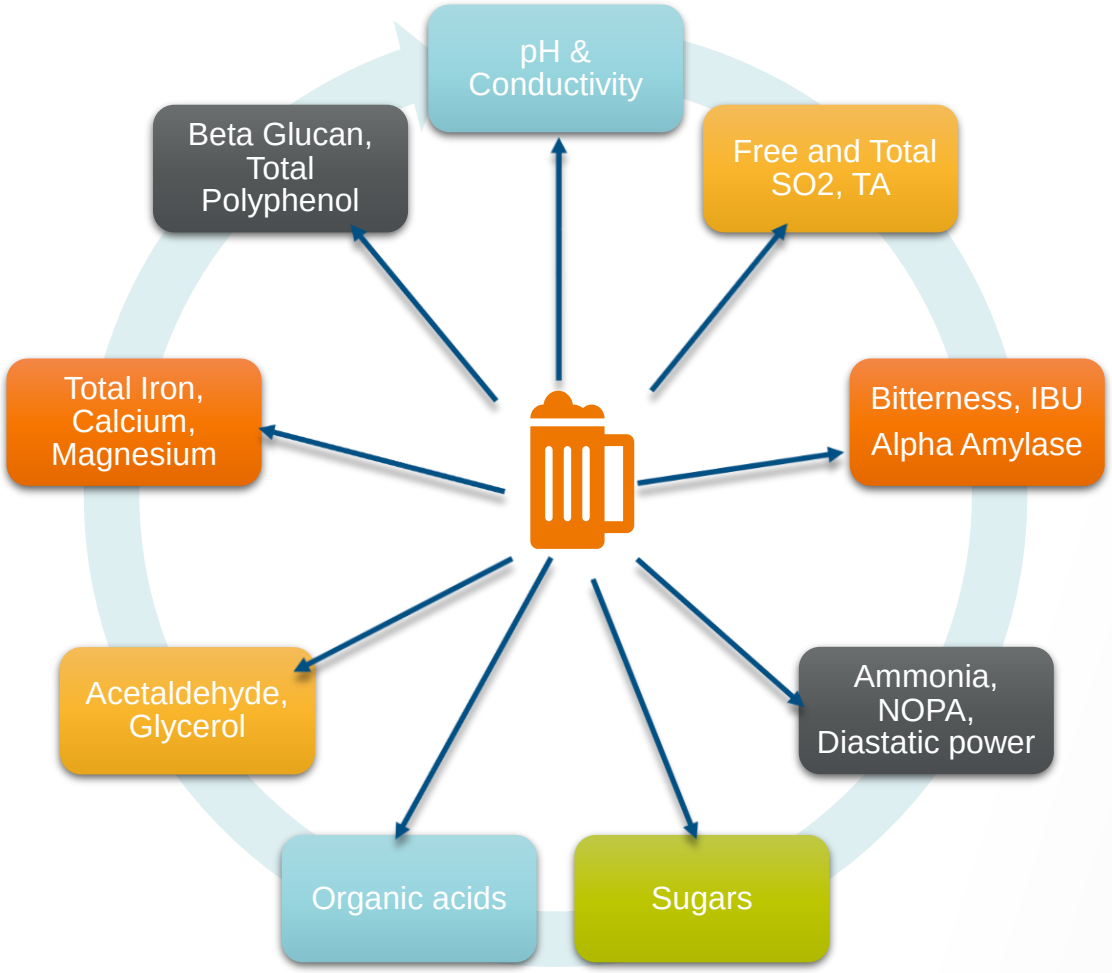
Example: malt & beer analysis



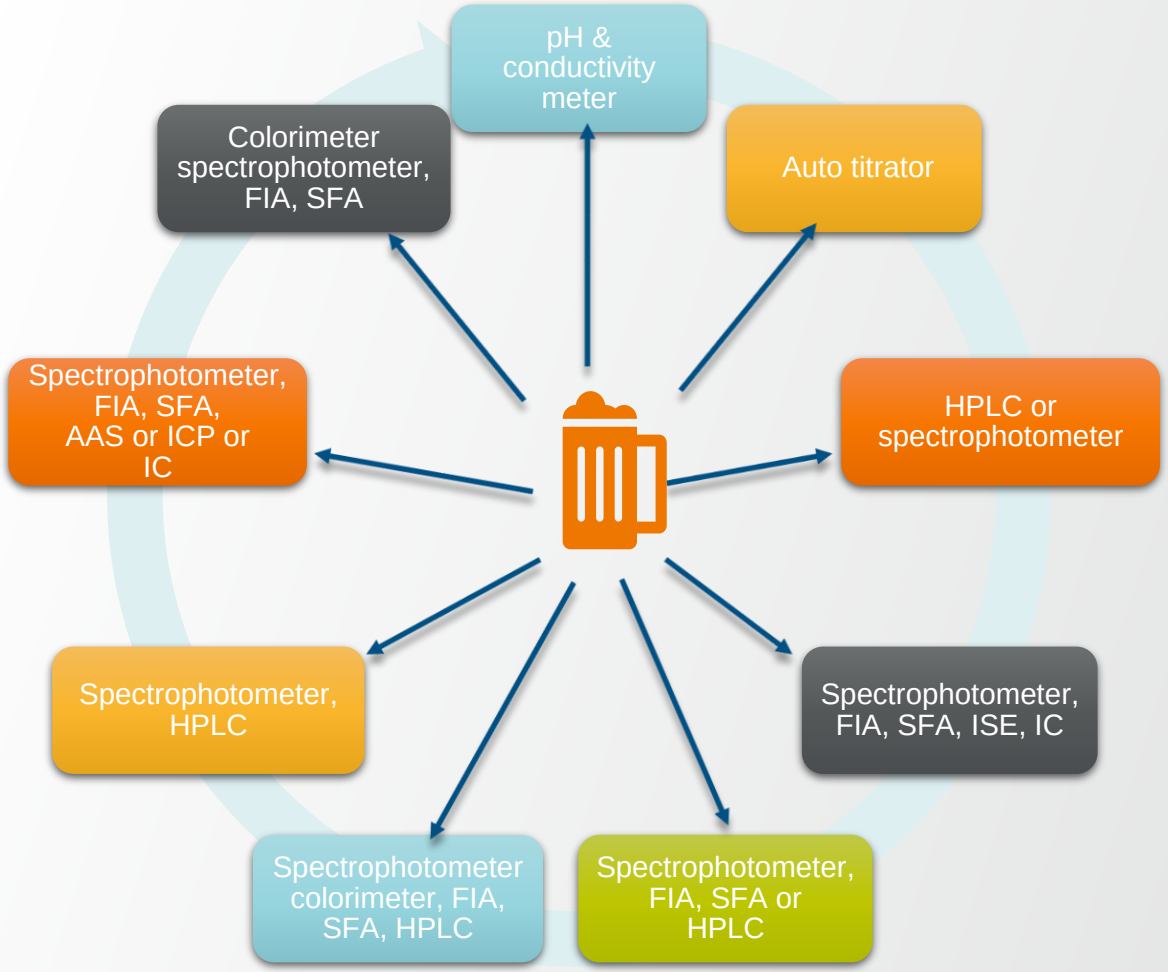
Example: wine analysis



Traditional analysis – multiple parameters, multiple instruments



Multiple parameters



Multiple techniques & instruments

Single instrument – single operator – multiparameter

Multiple parameters – Multiple instruments - Multiple operators

Single instrument – Single operator – Multiple parameters

What is wet chemical colorimetric analysis?

For a basic assay, in this case sulphate

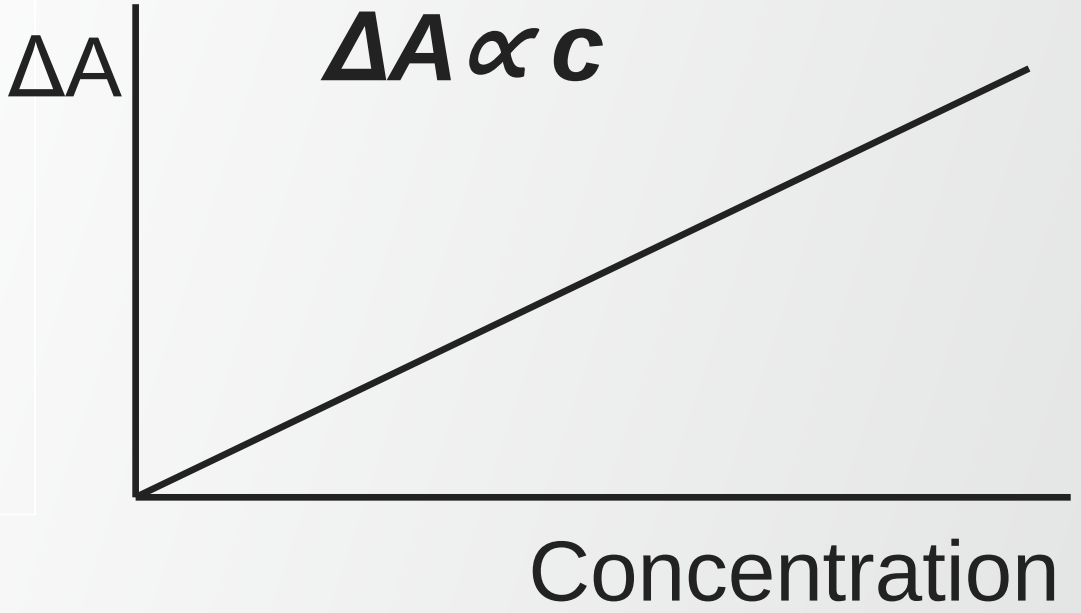
- Add an aliquot of sample (100µl)
- Shine light (420 nm) through the sample and measure the intensity in absorbance units (Au)
- Add an aliquot of barium chloride reagent (40 µl)
- Wait for the reaction to occur (300 s)

  [SO_4^- + BaCl = BaSO4 + Cl^-]
- Shine light (420 nm) through again and the difference in intensity is the change in absorbance ΔA

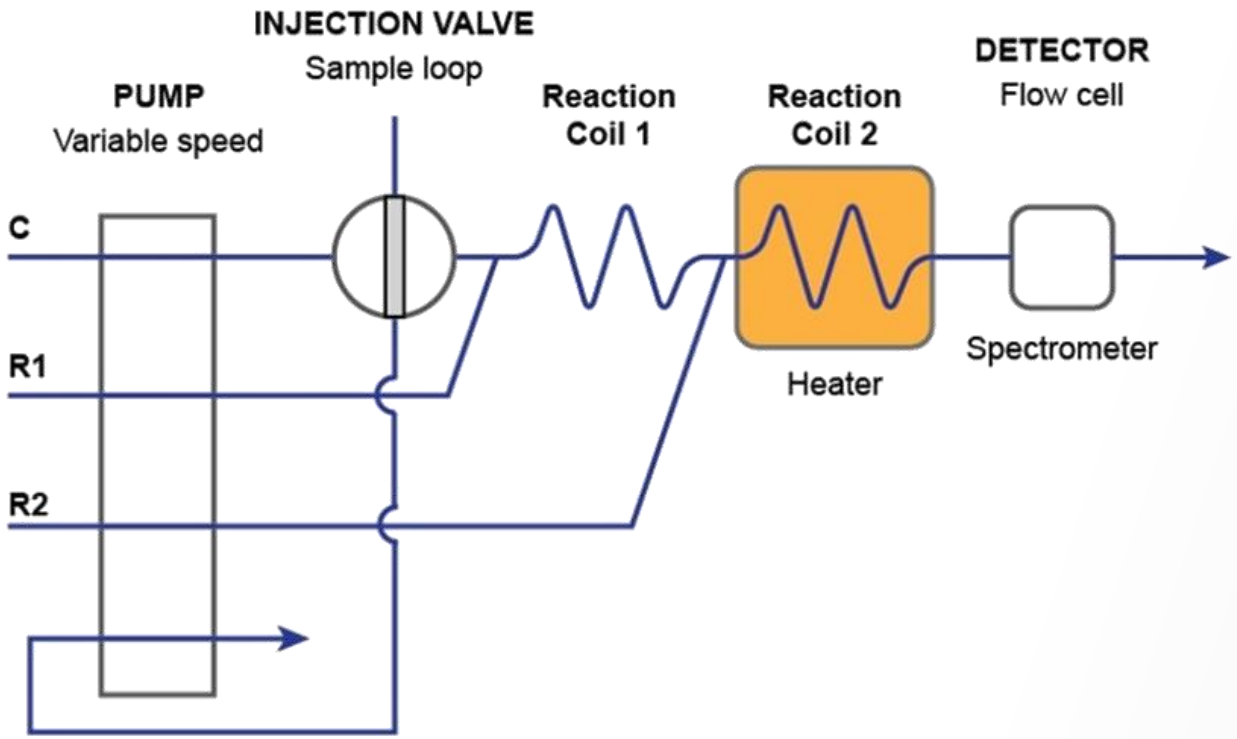
Beer–Lambert law

$$\Delta A = \varepsilon \times l \times c$$

$$\Delta A \propto c$$

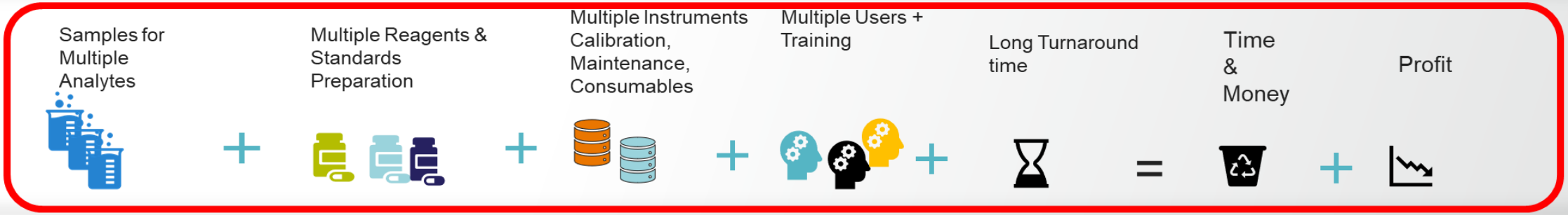


Traditional colorimetry workflow (CFA)



Continuous flow analyzers (CFA)

- Sequential instrument, one sample at a time
- Single analyte per system line
- Max 4 lines per system, multiple instruments
- 10-50 mL of sample required per test
- 10-50 mL of reagents required per test
- Liters of waste generation
- High cost per analysis



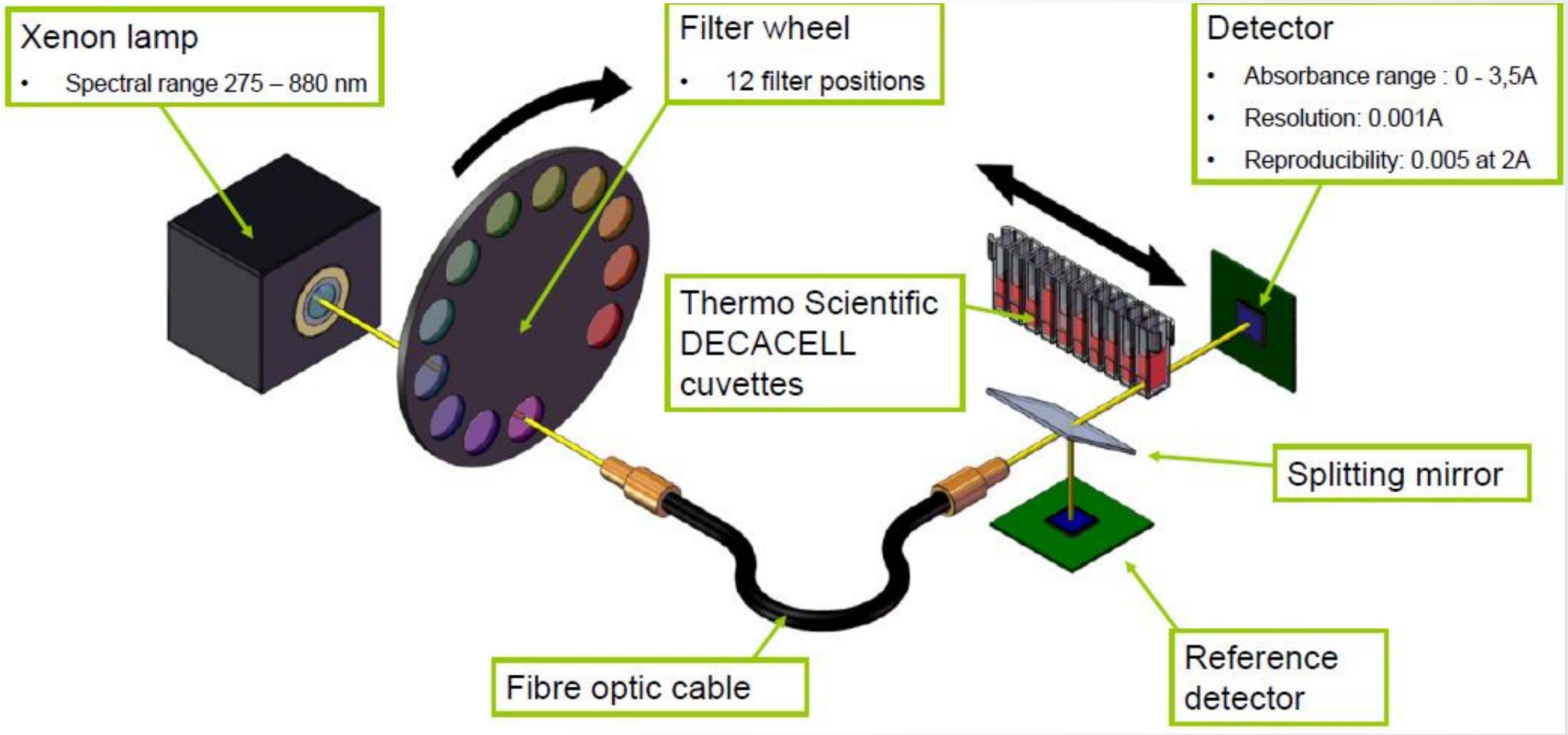
What is discrete industrial analysis?

Improved results reliability

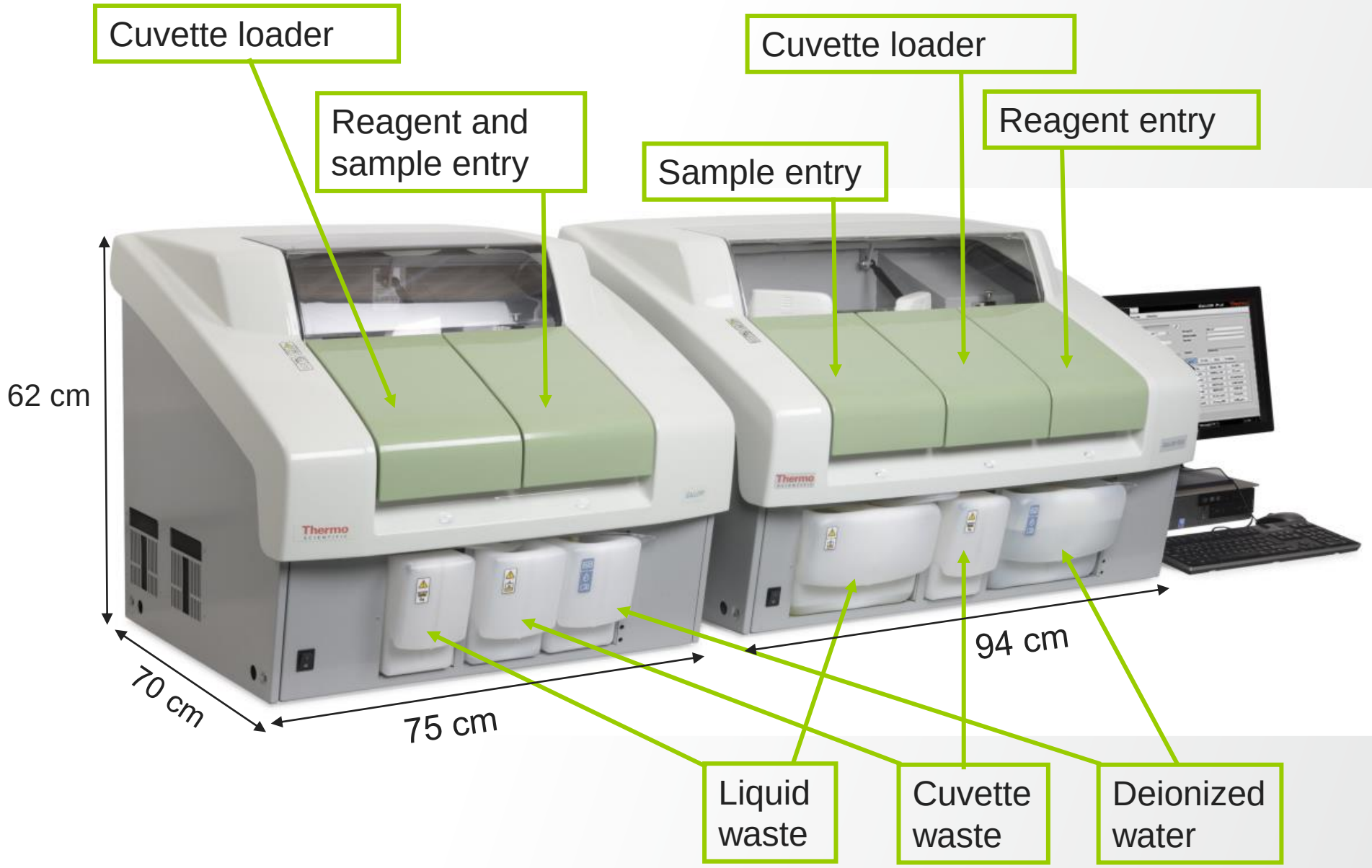
- ✓ Disposable discrete cells: peace of mind
  - Precision and accuracy
  - Improves throughput: no need for cleaning
  - No carry over
  - Wide range of chemical parameters
- ✓ Reliable results across wide concentration range
- ✓ Out of limits - flagged results
- ✓ QC check
- ✓ Low volume cuvette
  - Reduced sample and reagent consumption: 2-240 µL
  - Lowest waste generation and disposal cost
  - Reduced cost per analysis

Unique low volume Thermo Scientific™ DECACELL™ Cuvettes - practical advantages

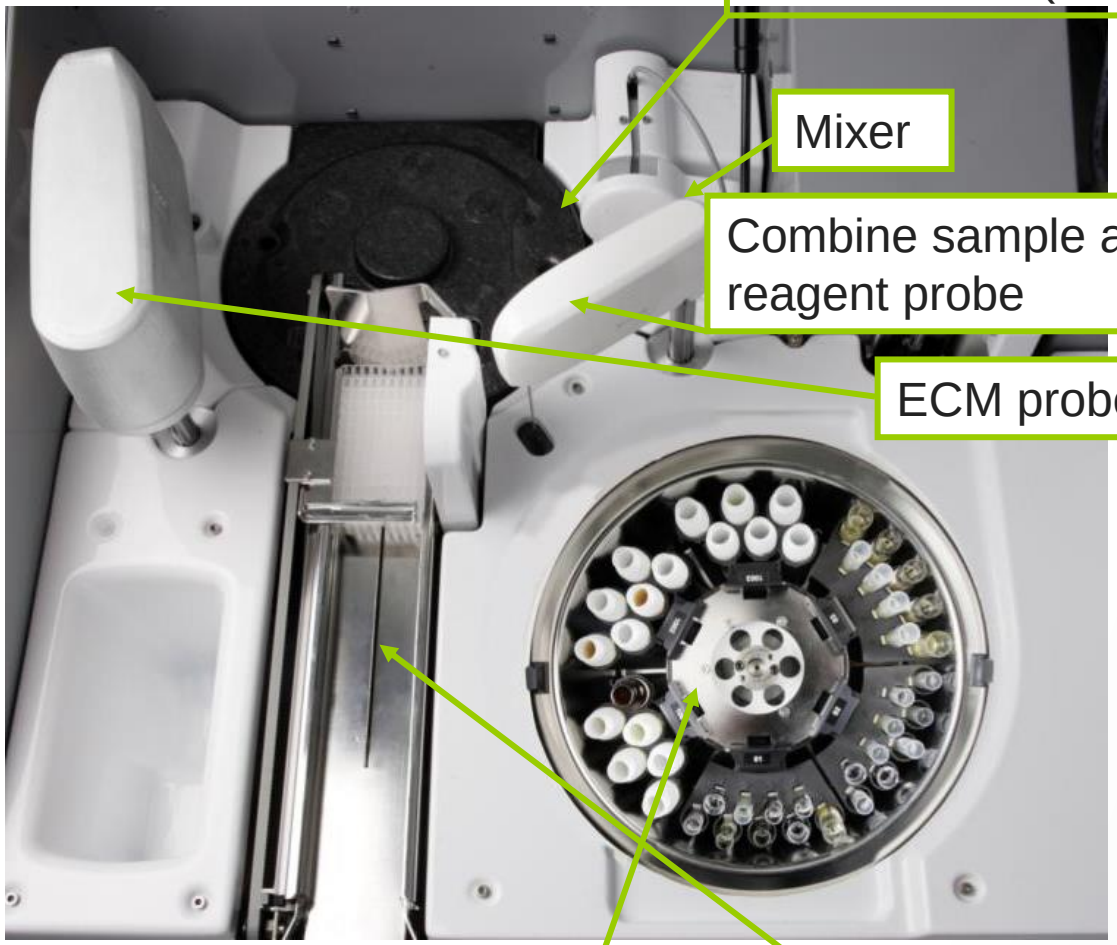
How does a discrete analyzer work?

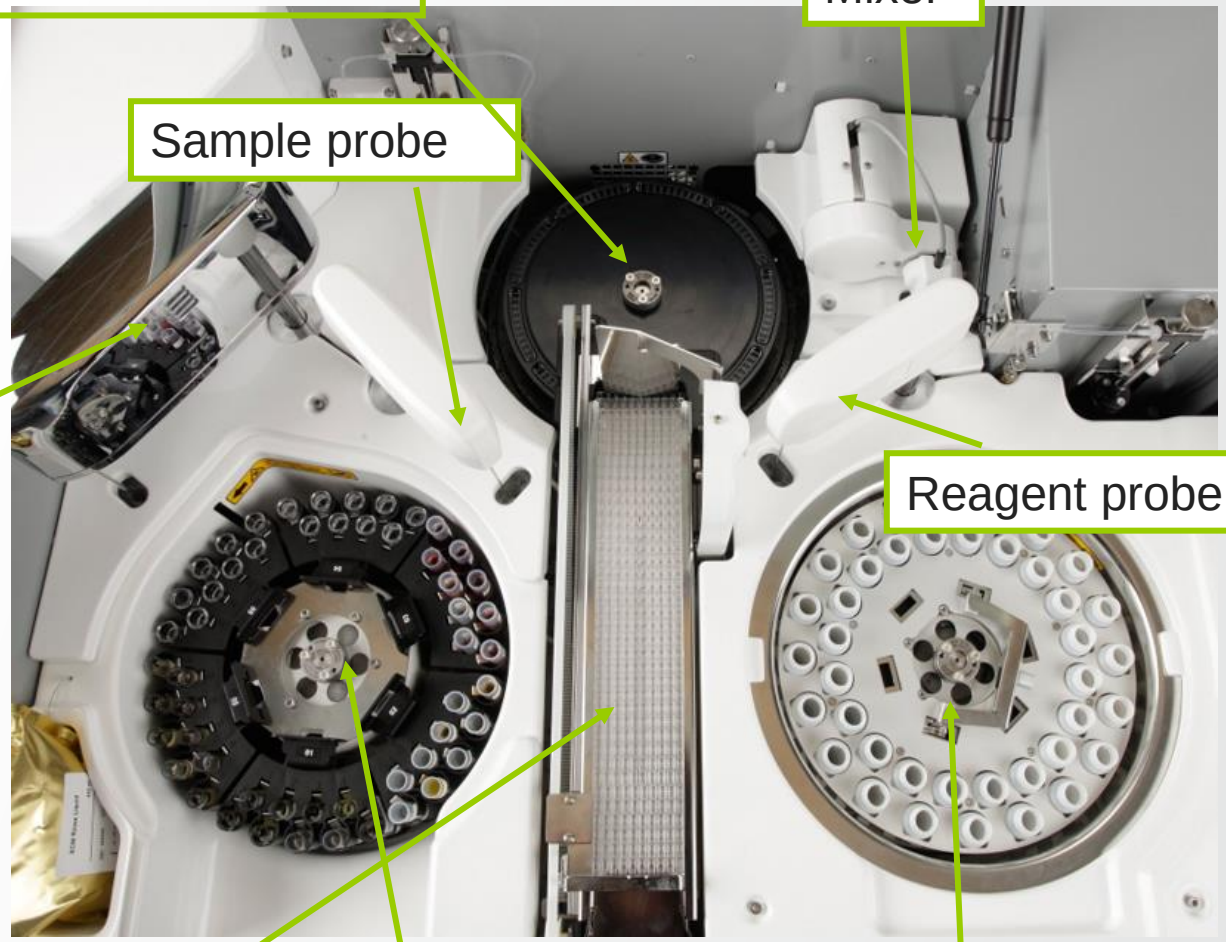


Thermo Scientific Gallery™ and Gallery Plus™ discrete analyzers



Inside the Gallery and Gallery Plus





Incubator – 9 (x10) DECACELL cuvettes

Mixer

Combine sample and reagent probe

ECM probe

Sample probe

Mixer

Reagent probe

Combine sample/reagent disk
6 sample or reagent racks

Cuvette storage – 36 (x10)
DECACELL cuvettes

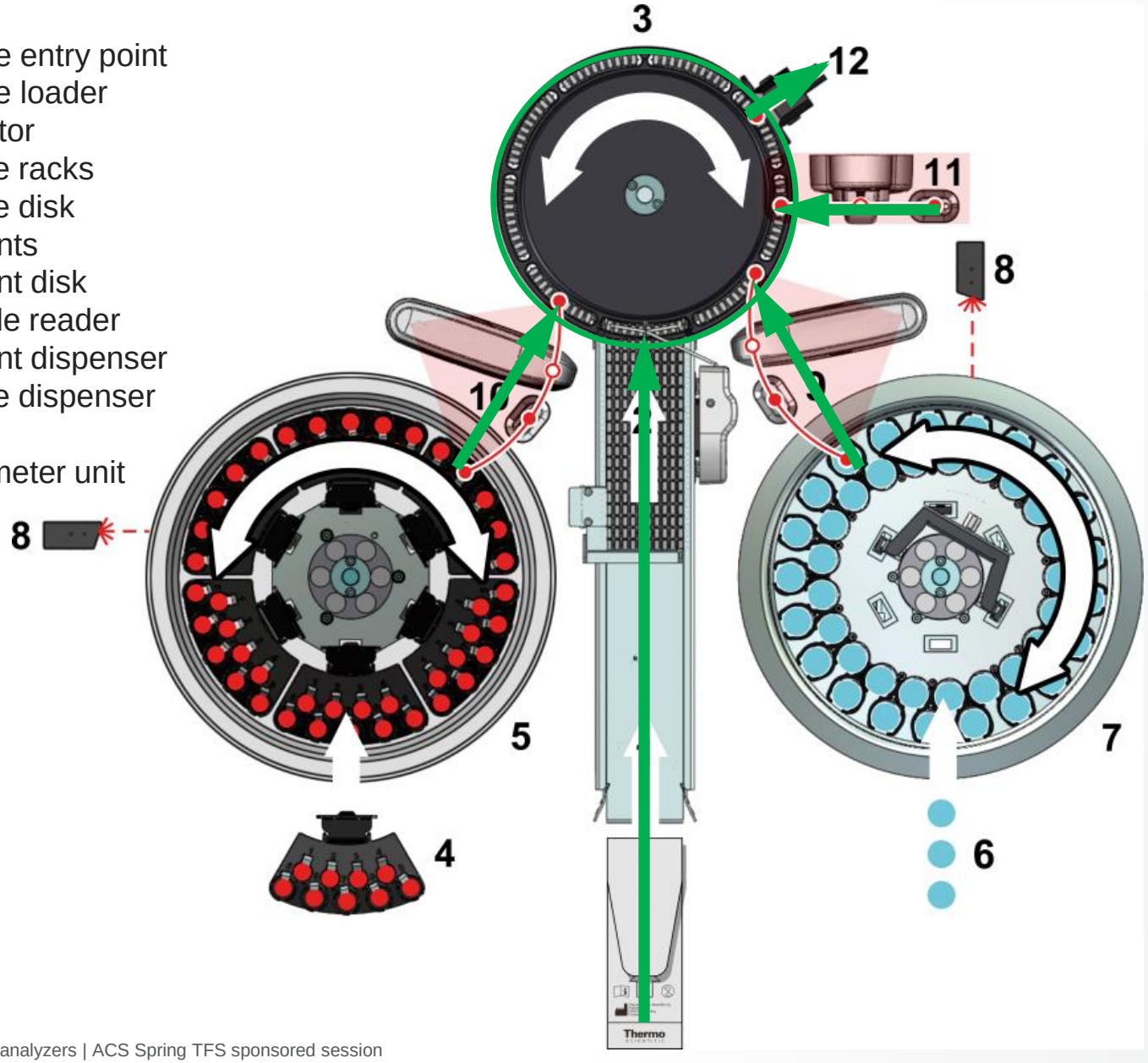
Sample disk
6 sample racks

Reagent disk
42 positions

How does the Gallery discrete analyzer system do it?

Key:

1. Cuvette entry point
2. Cuvette loader
3. Incubator
4. Sample racks
5. Sample disk
6. Reagents
7. Reagent disk
8. Barcode reader
9. Reagent dispenser
10. Sample dispenser
11. Mixer
12. Photometer unit



1. A cuvette is loaded from the cuvette loader (2) into the heated incubator (3)
2. The sample dispenser (10) an aliquot of sample from the sample rack (5) into a single cell of the cuvette
3. An initial measurement is made by the photometer (12)
4. An aliquot of reagent is dispensed from the reagent disk (7) via the reagent dispenser (9)
5. The mixer is used to mix the samples and reagents in each cell
6. The reaction is left to occur in the heated incubator (3)
7. A final measurement is made by the photometer (12) and the change in absorbance is calculated

Simplified workflow solution

Photometric detection

- Colorimetric
- Enzymatic
- Electrochemistry

Liquid handling

- Sample aspiration
- Reagent addition
- Mixing and washing
- Calibration, QC, spiking, and dilution
- Incubation

Automation

- Random access
- Parallel analysis
- Auto-dilutions on overrange samples
- High throughput

High throughput photometric analyzer

Automation enables a simplified workflow

Gallery discrete analyzer workflow

Load cuvettes

Insert samples

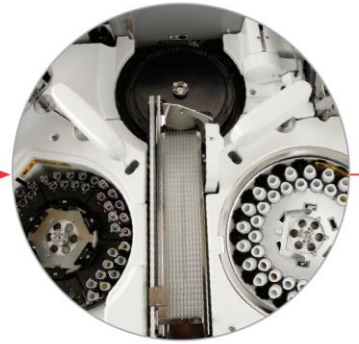
Insert reagents

Run analytes

Import sample table from LIMS

Create run table

Start analysis



Parallel pH/conductivity

Dispensing

Mixing

Incubation

Photometric measurement

Consolidated report

PDF

LIMS export

Spreadsheet

Walk away from Gallery discrete analyzer

Gallery Discrete Analyzer platform

Ease of Use, Low Training Requirement

new users can be trained in 2 days

Cost Effective (20x lower cost per test)

Lowest reagent, sample consumption, waste generation

Simultaneous Multiparameter Analysis

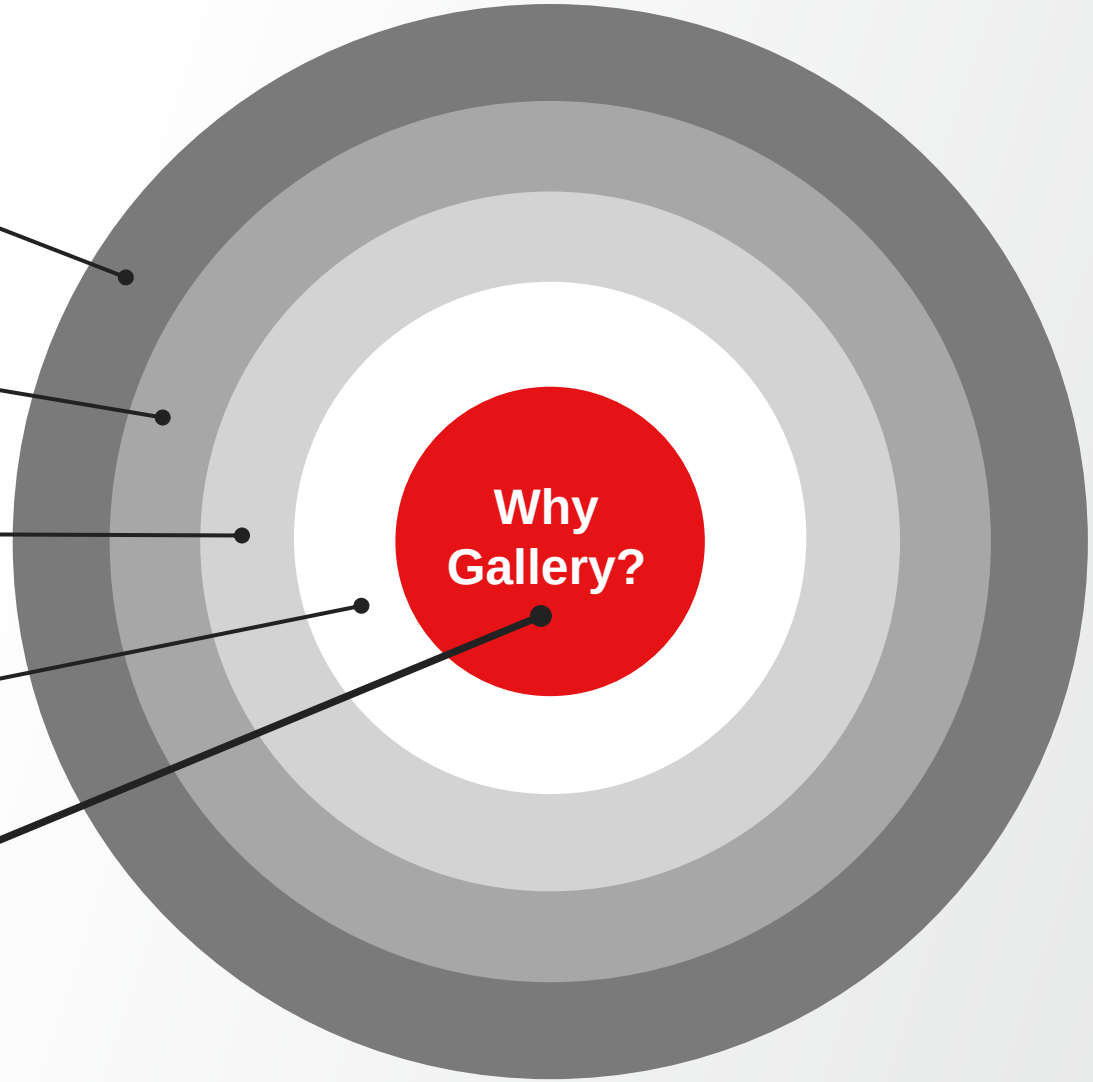
Up to 20 parameters per sample

Flexible & Open Systems

Open to 3rd party reagent, easy to adopt photometric test methods

High Throughput & Automation

Up to 350 Tests/Hr; parallel pH & conductivity, up to 3 hrs unattended operations



Automated wet chemical analyzer to speed up your scientific research

General comparison

	Automated discrete analysis	Segmented flow analysis
Cost of entry	low	high
Flexibility of system	high	Low
Hands on maintenance	lower	higher
Reagent volumes	small	large
Sample volumes	small	large
Training Requirement	Lower	higher

General comparison

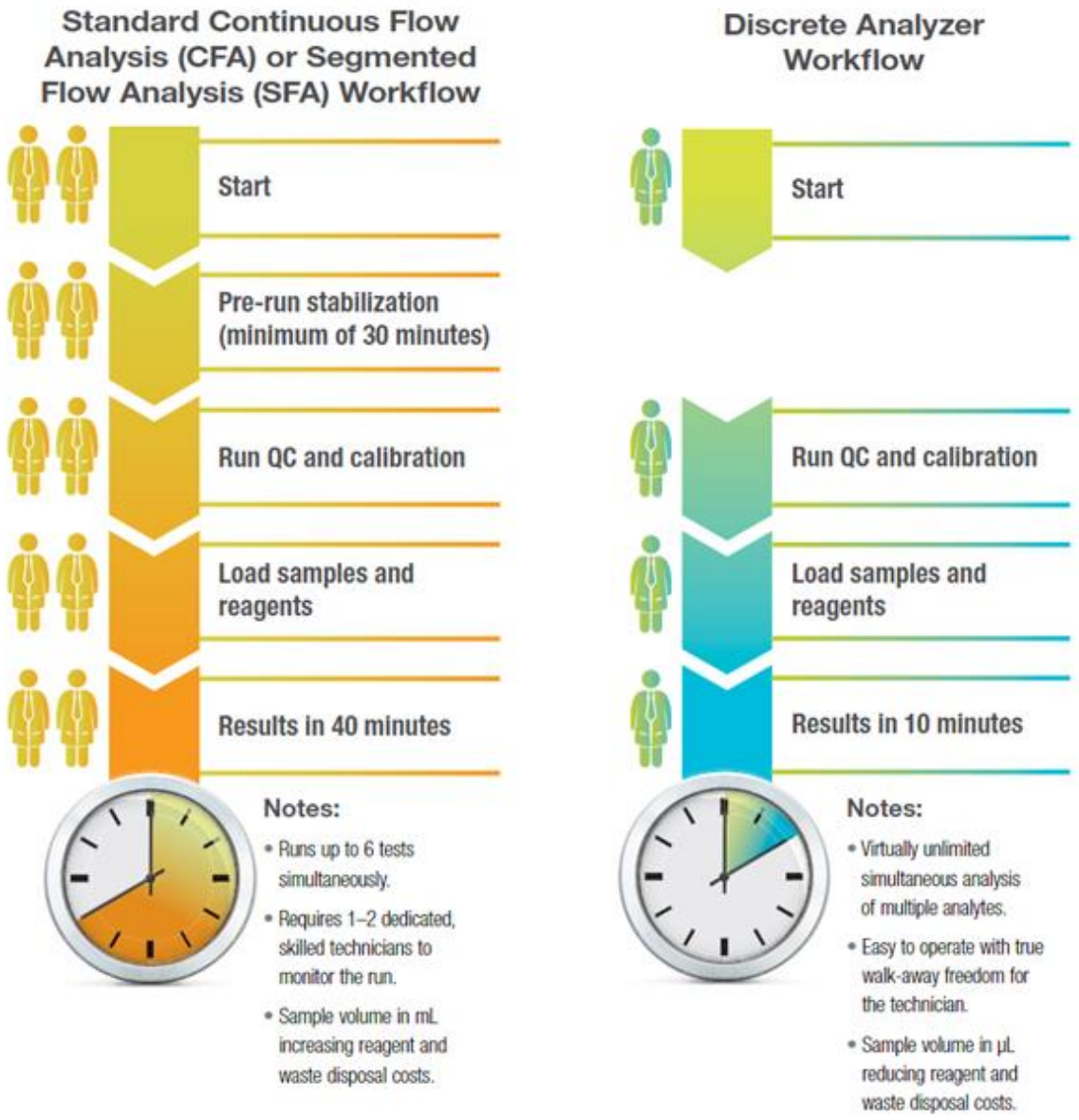
Traditional Wet Chemistry

- mL reagents
- 50–100 mL samples per test
- Liters of waste generation
- Multiple instruments
- Labor intensive
- Sequential or batch
- Typically single or max 4 parameters per sample
- Higher cost per analysis
- Low throughput: 20–80 tests/hr

Gallery Discrete Analyzer Platform

- 2–240 µL reagents
- Max 300 µL per test
- Few mL of waste
- Single platform
- Easy to operate
- Fully automated
- Parallel and batch
- Up to 20 parameters per sample
- Reduced cost per analysis
- High throughput 200–350 tests/hr
- Integrated barcode reader for samples and reagents

General comparison



Real world use experience – malt analysis

Montana State University, USA –Barley, Malt & Brewing Quality Lab

Quality attributes of beverage testing by integrated wet chemical analyzer

Hannah Turner | Director Barley, Malt & Brewing Quality Lab

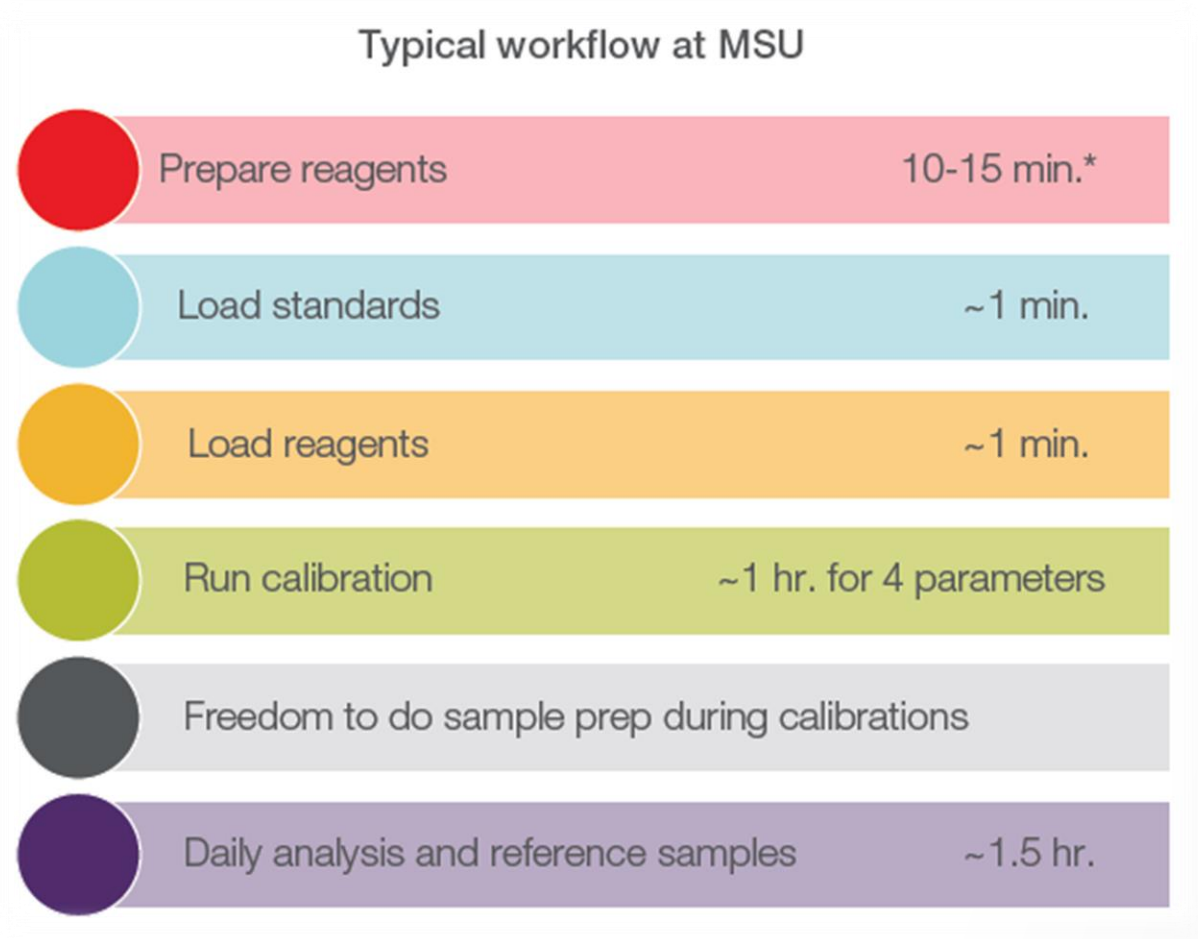
Hannah.turner2@montana.edu

MSU's Gallery Setup

- Gallery Discrete Analyzer - Basic
  - Capacity for 6 racks – shared reagent and sample storage
    - Typically 1-2 reagent racks & 4-5 sample racks
    - Sample racks = 18 samples each
    - Reagent racks = 6 reagents each
  - Temperature: 37 °C
  - Wavelengths:
    - 275, 340, 405, 430, 510, 520, 540, 575, 600, 660, 700, 880
- Annual maintenance contract
- Typical daily run: 32 samples (31 unknown/1 control)

Information courtesy of Montana State University's Barley, Malt & Brewing Quality Lab, USA

Typical Workflow at MSU

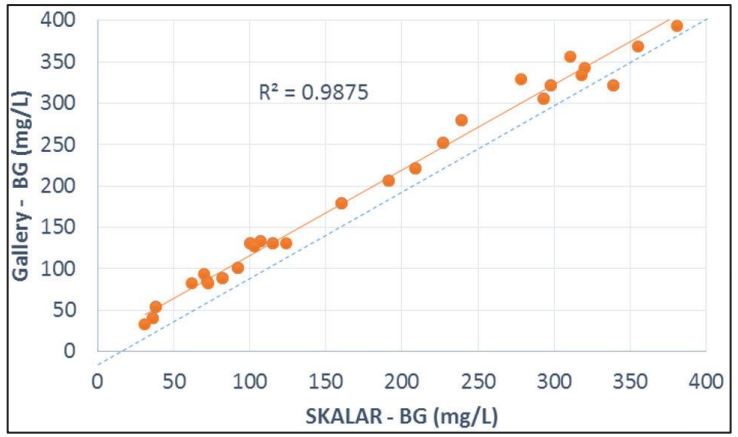


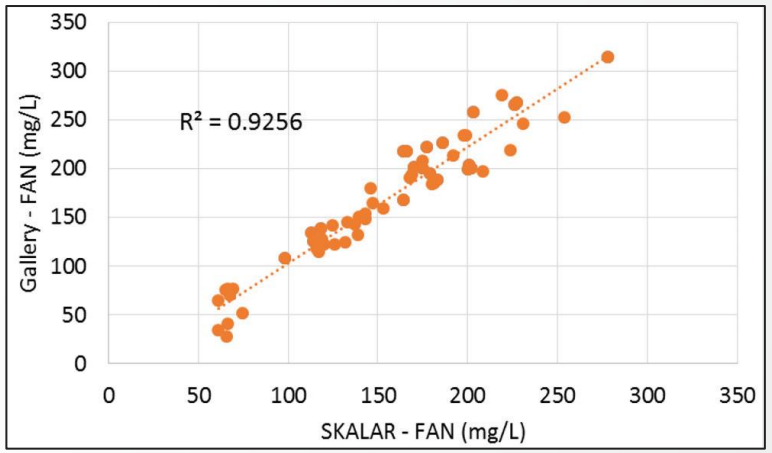
- High correlation with other industry standard analyzers
- Reduced set up time
- Reduced reagent volumes/cost
- Reduced sample size
- Robust analysis with high repeatability
- Open system for added flexibility

Information courtesy of Montana State University's Barley, Malt & Brewing Quality Lab, USA

High correlation to segmented flow analyzer

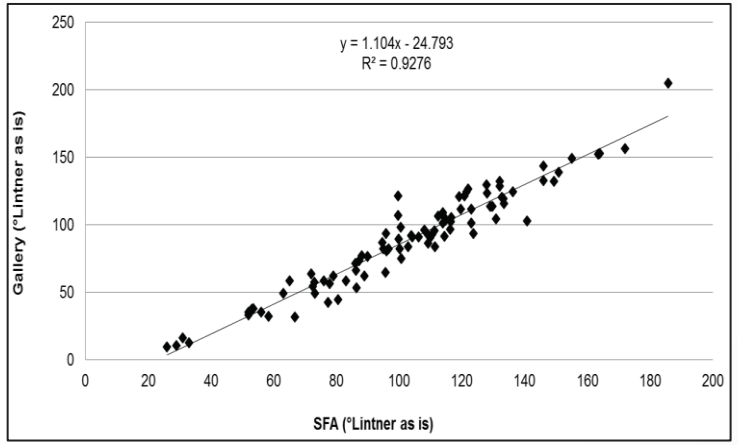
B-Glucan
R = 0.99

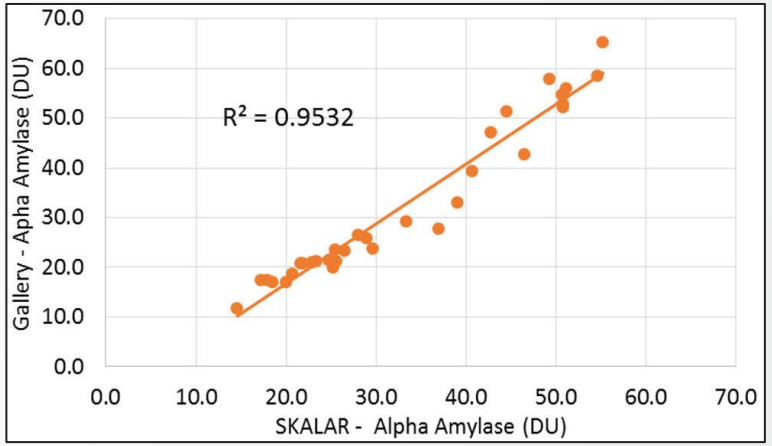




FAN (NOPA)
R = 0.93

Diastatic power
R = 0.93





A-amylase
R = 0.95

Data courtesy of Aaron Macleod & Montana State University's Barley, Malt & Brewing Quality Lab, USA

Automated malt analysis using discrete analyzers by Aaron MacLeod, Separation Science

ASBC ring test –published official methods

- Inclusion of labs across the US/Canada/Europe
- In 2020 the American Society of Brewing Chemists (ASBC) adopted the following **standard** malt analysis methods for discrete analyzer

Method Name	ASBC Official Method Number
Free Amino Nitrogen in Wort	Wort-12C
Wort Beta Glucan in Wort	Wort-18D
Alpha Amylase Activity in Malt	Malt-7E
Diastatic Power of Malt	Malt-6D

Conclusions in the ASBC reports:

The Repeatability and reproducibility coefficients of variation for **Free Amino Nitrogen, β-glucan, alpha-amylase, and diastatic power**, in malt by automated discrete analysis were **judged acceptable** and **similar to** the results from a previous collaborative study using the segmented flow analysis method.

Sources: AMERICAN SOCIETY OF BREWING CHEMISTS, INC. Report of SubCommittee

Real world use experience – inorganic fertilizers

Evira, the Food Authority located in Helsinki, Finland

Issues the Food authority was facing:

- The lab at Evira routinely measures potassium (K) and phosphate (PO4) for approximately 1000 inorganic fertilizer samples per year. The analysis used to consume two days with old titration and gravimetric methods.

Tests of interest:

Potassium, phosphate, chromium VI

Precise analysis for inorganic fertilizers at the FInnish Food Authority (thermofisher.com)

Precise analysis for inorganic fertilizers at Finnish Food Authority

Evira –Helsinki, Finland

Benefits identified by Evira

- In two hours they are able to complete all the required analyses using the Thermo Scientific™ Gallery™ automated discrete analyzer. The same analysis used to consume two days with old titration and gravimetric methods
- “Phosphate samples are not an issue with the Gallery analyzer and there is no glassware to clean. I hate cleaning glassware”
- For the K test, the existing method was modified to accommodate a range of 40–1000 mg/L
- Has also measured chromium VI (CrVI) from living compounds using the Gallery discrete analyzer
- the Gallery discrete analyzer has ensured faster analysis while allowing them to maintain the precision they require for compliance with government regulations

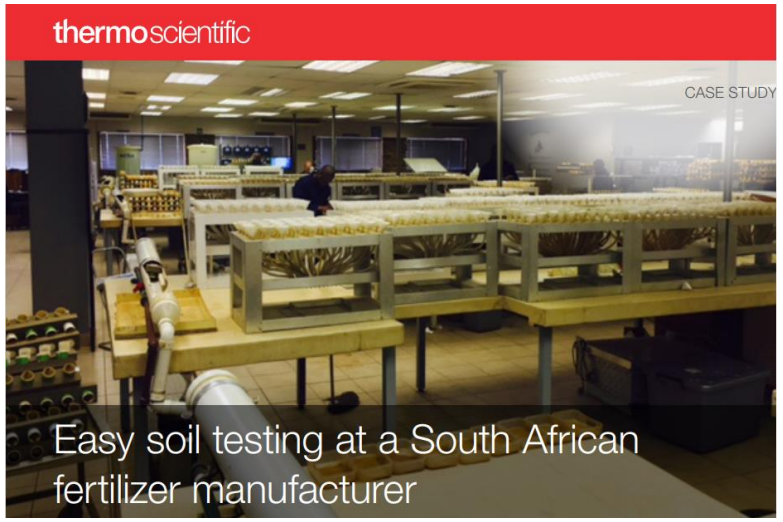
> “This is the best method for measuring PO_4 in inorganic fertilizers. It is much more precise since there is no interference from other analytes.”
>
> —Aija Pelkonen,
> Research Chemist, Evira

Real world use experience – soil testing

Omnia Fertilizer, South Africa whose R&D department advises and provides tools so farmers can improve practices

Issues the R&D department of Omnia was facing:

- In the past, the R&D lab used a Segmented Flow Analyzer (SFA) to measure soil phosphate and nitrate via bray 1 extract method in soil sample matrix.
- With 4000 samples to test each day during the May to October growing season, balancing the operation of multiple SFA instruments and lines was a tedious process over 4 shifts
- Using SFA equipment required several operators as well as the expertise of a specialist who could not only operate the instrument but troubleshoot the problems
- The equipment regularly experienced long downtime maintenance or service issues.
- A lot of chemical waste was produced each day, typical days would produce 15-25 L



Tests of interest:

Phosphate w/ soil bray 1 extract (good pH control)
total nitrogen (vanadium), Mehlich III Phosphorus (P) in soil
potassium (K), Ammonia, Chloride

Easy soil testing at a South African fertilizer manufacturer

Omnia Fertilizer, South Africa

To solve their problems, the managers of the lab purchased 8 Thermo Scientific™ Gallery™ discrete analyzers throughout the years.

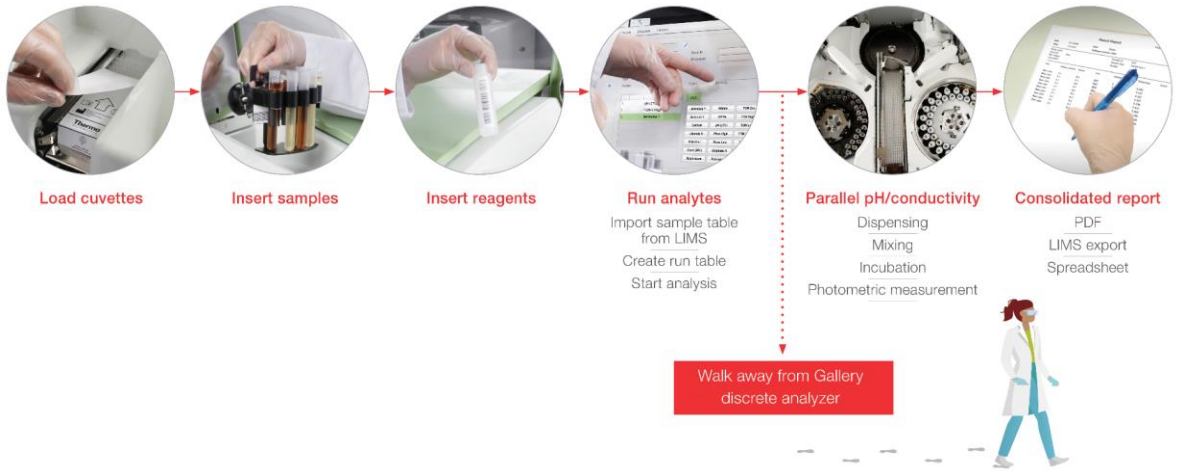
Benefits identified by Omnia

- Accuracy, precision and reproducibility with the discrete analyzers was directly comparable to the SFA results
- Operator friendly, each instrument is simple to use by a single technician. 4 shifts schedule reduced to 2 shifts with significant time saved.
- No need to separate out sample preparation to separate instruments, all tests for each sample could be analyzed on a single instrument
- Chemical waste production was typically 2-5 L per day, which included all dispensing and diluent water, allowing it to be disposed of as a lower tier waste

> "Maintenance is substantially less than with our older test methods."
>
> —Edna Laubscer,
> Chemtech Analytical Services Manager, Omnia Fertilizer

Ease of use

Walkaway efficiency



- ✓ Automated start up and shutdown
- ✓ Barcode readers for both samples and reagents
  - ✓ Eliminates manual errors
- ✓ Easy to build sample run table
  - ✓ Import from LIMS
  - ✓ Import from csv file

- ✓ Low training requirements for lab technicians and operators
- ✓ Easily expandable
- ✓ Resolves lab staffing issues and improves productivity
- ✓ Enables lab technicians with more time to focus on other important tasks

Flexible & open systems

- ✓ Open to 3rd party reagent for more method development, and you can continue to use your own prepared reagents
- ✓ Versatile to modify existing methods
- ✓ Easy to transfer existing segmented flow test methods or spectrophotometric methods

Ready-to-Use Reagent Kits

Peace of mind

- ✓ Ready-to-use liquid reagents eliminate reagent preparation
- ✓ Provide tracability and peace of mind with CoA (Certificate of analysis)
- ✓ Save operator time with ready-to-use liquid reagents
- ✓ Minimal reagent waste
- ✓ Bar-coded reagent vials provide easy and reliable identification
  - ✓ Lot, expiration date information
  - ✓ Real-time reagent monitoring

Multiparameter & high throughput Analyzer

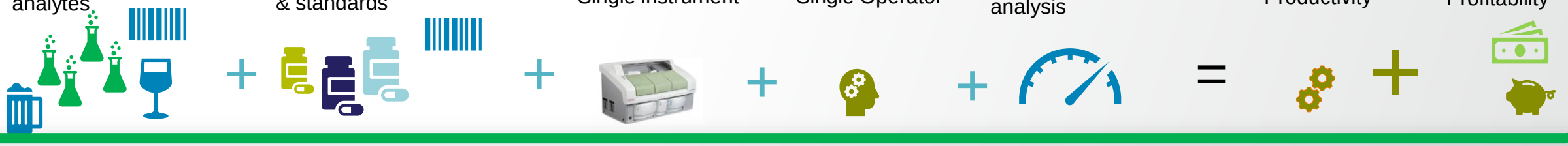
Increased productivity to speed up your research progress

- ✓ Capable of performing simultaneous photometric and parallel electrochemistry (pH and conductivity) measurements. Up to 20 parameters per sample
- ✓ Capable of performing 200 -350 tests/hr
- ✓ Improvement in precision vs. traditional wet chemical testing techniques

Integrated multiparameter analyzer – Gallery Discrete Analyzer

Samples for multiple analytes + Multiple reagents & standards preparation + Multiple instruments calibration, maintenance, consumables + Multiple skilled technicians + Long turnaround time = Time & money + Profit

Samples for multiple analytes + Ready-to-use reagents & standards + Single instrument + Single Operator + Fast multi parameter analysis = Productivity + Profitability



Voice of the customers

Gallery Users Testimonials

"An excellent correlation to existing flow injection analysis and manual methods, a short training period, reduced hands on time when analyzing the samples and a short time to result with Gallery and Gallery Plus instruments are clear advantages."

Henrik Lindblom
Laboratory Manager, VA SYD, Sweden

"It would take an entire day in the past to complete seven tests on eight samples using traditional wet chemistry methods. Now 50 tests are completed in one hour."

Paul Taylor
Laboratory Manager
Murphy and Son Limited

"The Gallery analyzer has reduced our stress level. We can put samples in the analyzer and walk away where we used to be tied to a measurement timing every ten minutes."

Jaana Pajulahti-Kiuru
Laboratory Technician, Fazer Group

Learn more about Gallery systems

Visit **www.thermofisher.com/discreteanalysis**

- 3D Product Tour
- Technology overview
- Educational videos
- More on-demand webinars
- Smart note, application notes, brochures
- Reagent information

Come and join our technical session on Wednesday to learn more about water and soil testing with the improved and new Gallery Aqua Master systems

PAPER ID: 3814395
PAPER TITLE: Automated simultaneous multi-parameter wet chemistry testing using improved discrete analysis technology
DIVISION: Division of Analytical Chemistry
SESSION: Advances in Spectroscopy
DAY & TIME OF PRESENTATION: Wednesday, March 29, 2023 from 4:40 PM - 5:05 PM
ROOM & LOCATION: Kentucky - Indianapolis Marriott Downtown

Thank you