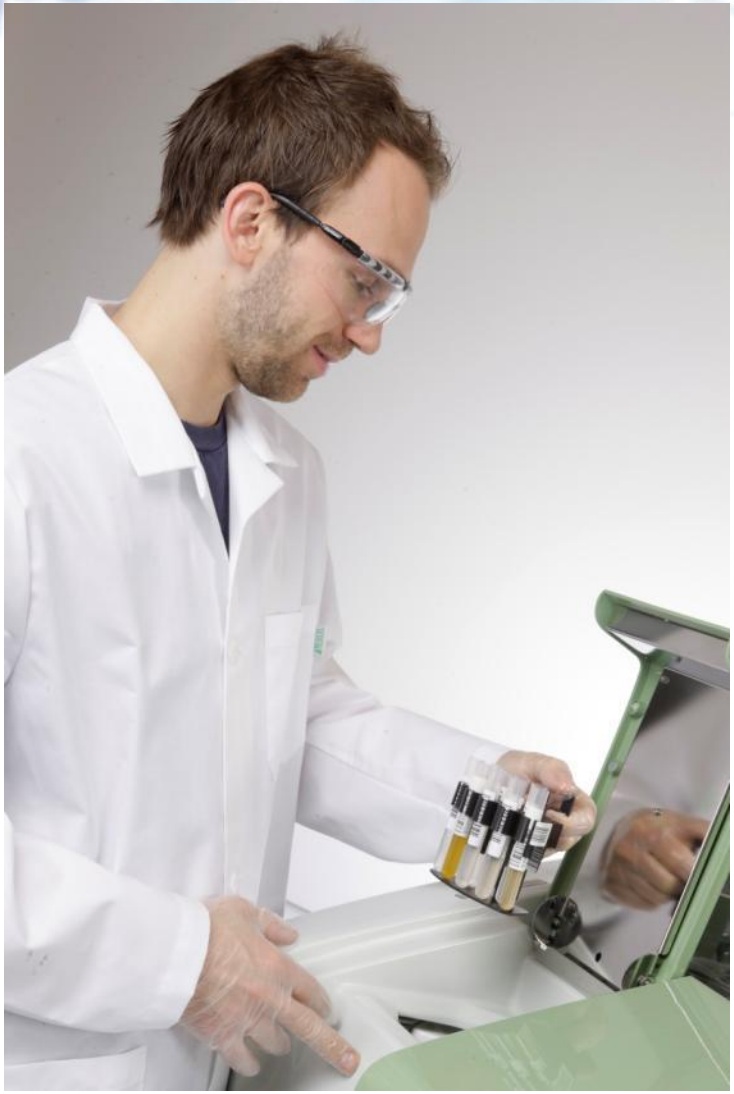
Applications for Discrete Analyzers

Thermo Fisher Scientific
Sunnyvale, CA

Discrete Analyzers – Outline

- What are Discrete Analyzers
- Where are they used
- What tests can a Discrete Analyzer perform
- Example Applications

What are Discrete Analyzers



- Automated photometric instruments that quickly perform a broad range of tests
- Individual tests for specific analytes covering food and beverage analysis, water and environmental testing, and quality control
- Accurate and precise colorimetric, enzymatic, and electrochemical measurements
- Powerful automated features to adapt applications to your specific needs

Benefits of Automated Discrete Analysis

- Flexible –
  - Multiple tests can be performed on a sample
- Fast –
  - Ready for immediate analysis: no reagent priming, no method changeover time
- Precise –
  - Specific measurements with high repeatability
  - Achieves ppb detection levels
- No carry-over –
  - Each reaction happens in its own disposable cuvette for contamination-free analysis
- Cost effective solution –
  - Low volumes of water and reagent used resulting in less waste for disposal

Gallery and Gallery Plus – Bench-top Analyzers

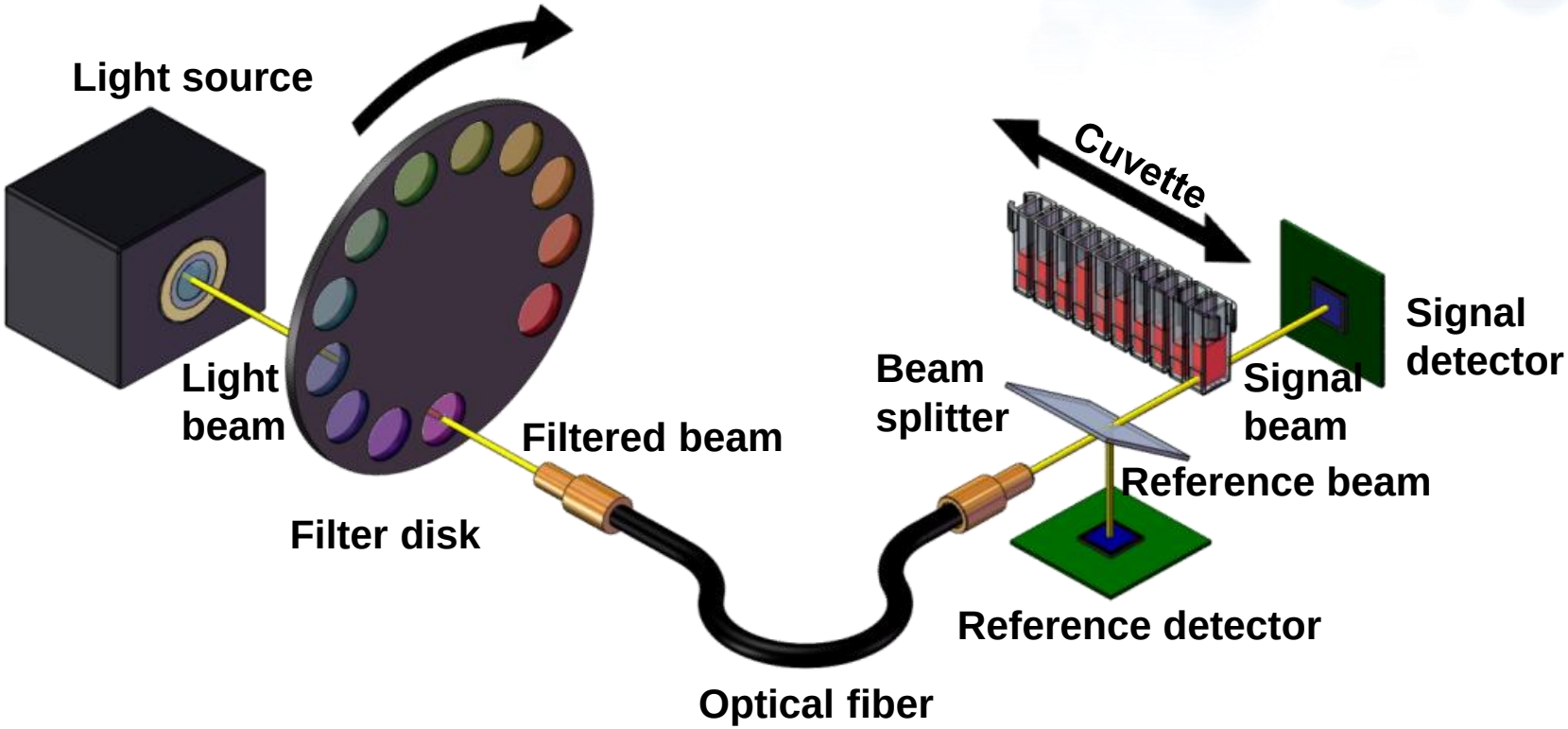
- An excellent automated platform for colorimetric, enzymatic, and electrochemical tests
  - All necessary analysis steps are automated
  - All tests performed in an easy and cost effective way

Maximum theoretical capacity with ready to use reagents:	up to 200 photometric tests/hr with Thermo Scientific™ Gallery™ analyzer	up to 350 photometric tests/hr with Gallery Plus analyzer

Gallery Plus System Description

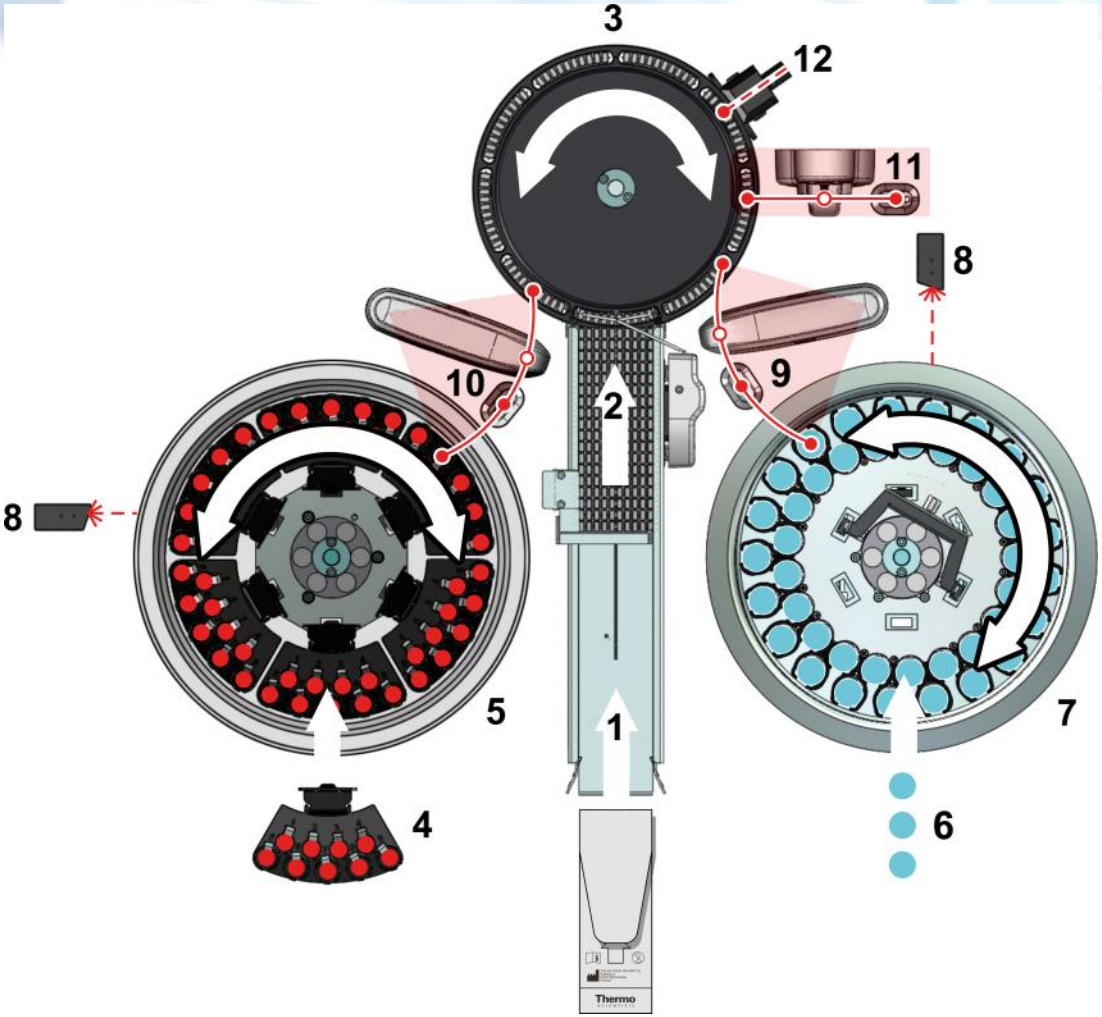
Photometric Principle and Measurement

- Spectral range 275 – 880 nm
  - 12 filter positions



Absorbance range : 0 - 3,5A
Resolution: 0.001A
Reproducibility: 0.005 at 2A

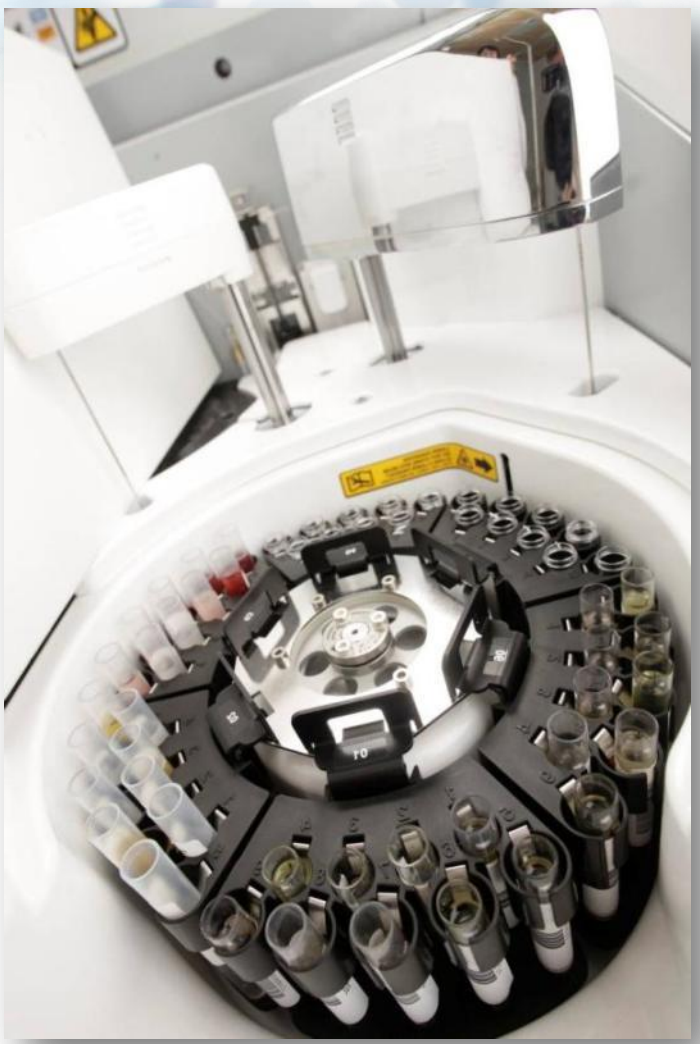
Discrete Analysis Process



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

Flexible Sample Management

- Sample volumes from 2 to 120 µL
- Any mix of sample containers
  - 0.5, 2.0 and 4.0 mL sample cups
  - 5.0, 7.0 or 10.0 mL sample tubes
- Automatic identification via an internal barcode reader
- Tests can be requested individually or by using a profile

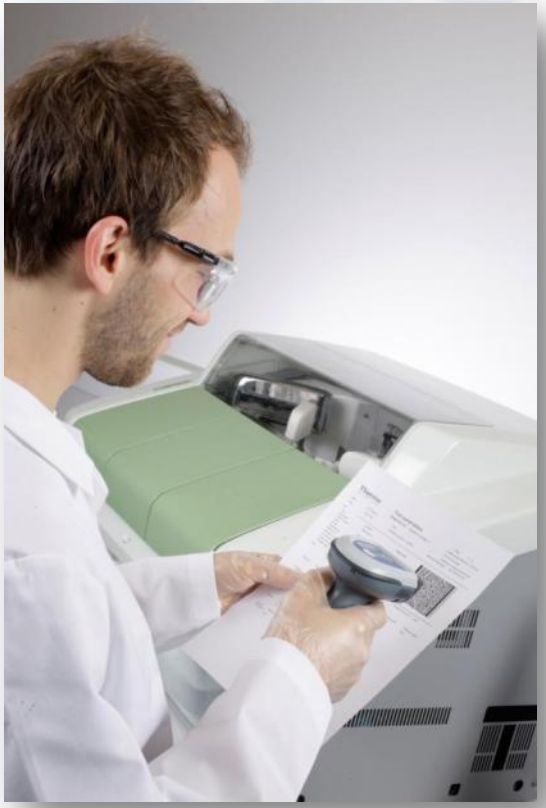


Comprehensive Data Handling

- Application parameter values readable from barcode or electronically from a file

- Results
  - Calculated from both measured and off-line results
  - Automatically flagged in case of
    - Abnormal values
    - Repeats
    - Out-of-limit control values

- Long term storage of results
  - Associated calibrations
  - Reagent lot data



Reporting Options

- Reports available
  - Spreadsheet export for further calculations
  - Export to LIMS
  - Printouts
  - PDF files

Calibration results

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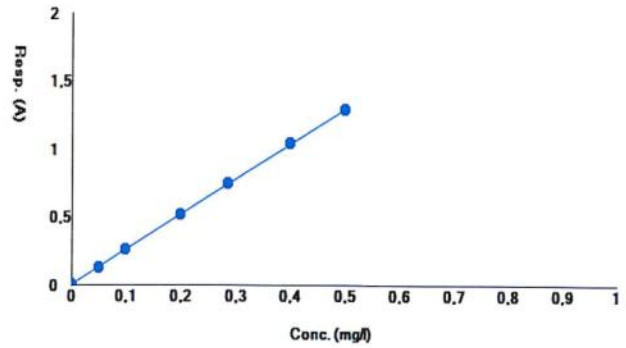
NO2 2mg/l Version number 1.4

Date	2014-02-17	User	Dealer
Time	12:53:25	Software version: 4.1.1	

Test	NO2 2mg/l	Coeff. of deter.	0,999956
Status		Total factor	0,387
Accepted	2014-02-13 10:36		
Checked	2014-02-13 10:36		
User name	Dealer		
Comment			
Errors			
Factor	0,387		
Bias	0,003		

Cal/Ctrl	Response	Calc. conc.	Given conc.	Lot	Errors
NO2-0	0,001	-0,001	0,000	Default	
NO2-STD	0,130	0,049	0,050	Default	
NO2-STD	0,260	0,100	0,100	Default	
NO2-STD	0,522	0,201	0,200	Default	
NO2-STD	0,743	0,287	0,286	Default	
NO2-STD	1,038	0,401	0,400	Default	
NO2-STD	1,288	0,498	0,500	Default	



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Discrete Systems - Markets

- Food/Beverage market
  - Fruit juice producers
  - Wineries
  - Breweries
  - Dairy companies
- Industrial bioprocess
  - Detergent manufacturers
  - Food additive producers
  - Enzymes manufacturers
- Water/Environmental market
  - Drinking water companies
  - Waste water plants
  - Government institutes
  - Commercial global companies






DA Food & Beverage Applications

Sugars

- D-Fructose
- D-Glucose
- D-Fructose+D-Glucose
- D-Fructose+D-Glucose+Sucrose
- Lactose (Glucose)
- Sucrose (Total)

Acid analysis

- Acetic acid
- L-Ascorbic acid
- ß-Hydroxybutyric acid
- Citric acid
- D-Gluconic acid
- D-Isocitric acid
- D-Lactic acid
- L-Lactic acid
- L-Malic acid
- Oxalic acid
- Tartaric acid
- Total acids

Over 50 optimized system solutions

Alcohol analysis

- Cholesterol Food
- Ethanol
- Glycerol
- Polyphenols (total)

Others

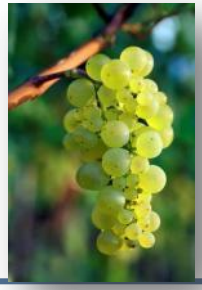
- Ammonia
- Acetaldehyde
- α-Amylase
- α-Amino Nitrogen (NOPA)
- Bitterness
- Beta-Glucan (High MW)
- Calcium (Ca)
- Copper
- Magnesium
- pH (Colorimetric)
- Potassium
- SO2 free and total
- Total Iron
- Total Protein
- Urea (Ammonia)

ECM

- pH

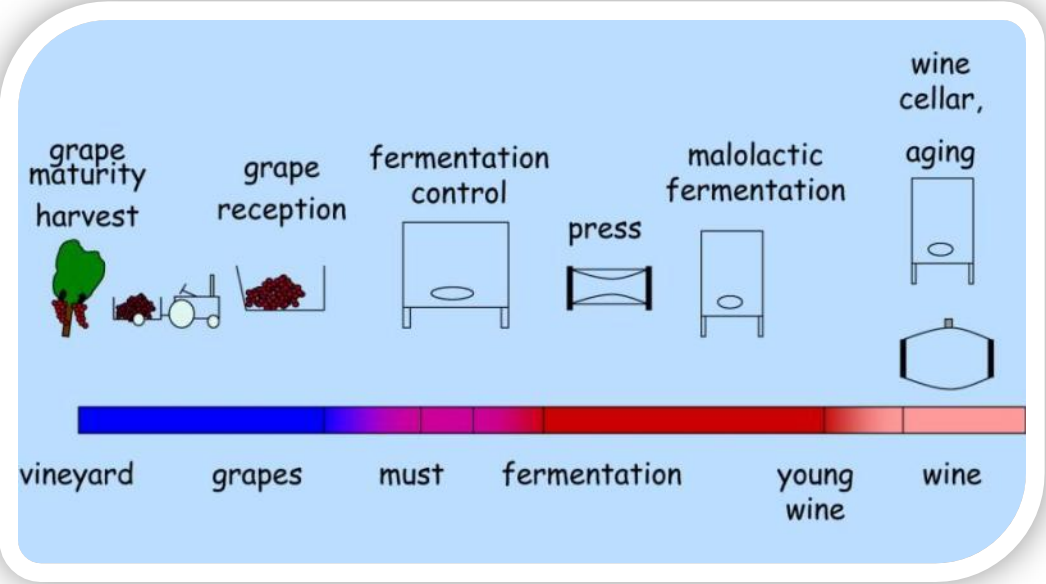
Calibrators

- Alcohol std
- Acetaldehyde std
- Acid combination std
- Beta-Glucan Std
- Beta Hydroxybutyrate std
- Cholesterol std
- Copper std
- Glycerol std
- Lactose std
- NOPA std
- Oxalic acid std
- Sugar combination std
- Urea std
- pH standards



Reasons for Beverage Analysis

- Quality Control of raw material, must (wine), or wort (beer), and final product
- Monitoring of production processes (malolactic fermentation)
- Detection of adulteration and false declaration
- Label claims /legal limits



Sugar and Acid Analysis in Wine

- In wine, fructose is used as a process indicator and a quality indicator for the final product
  - Yeast enzymes convert sugars (sucrose, glucose, and fructose) to ethanol and carbon dioxide
  - Sucrose is first converted to glucose and fructose, then glucose is consumed followed by fructose

- Acids play a significant role in taste, color, and microbial stability of juice. In wine, acids are present in both grapes and wine.
  - Acids, like D-Malic acid are tested to monitor the fermentation process

- Other tests for wine
  - SO_2 level regulated by legislation
  - Glycerol as a taste parameter

Sugar and Acid Analysis in Fruit Juice

- Sugars like sucrose, glucose, fructose and sorbitol are tested in raw materials and the final product

- Ratio of sugars from concentrate are used to verify authenticity
  - Glucose/ fructose ratio from apple juice
  - Citric acid/ iso-citric acid ratio from citrus juices

- Acids and alcohol are checked to monitor the level of natural fermentation – this limit is regulated by law

Ready-to-use Test Kit Analysis

- Kits include all reagents needed for each assay
  - Enzymes
  - Buffers

- Usually kits are ready-to-use and do not need additional preparation – just open the cap and use

Key Benefits of Thermo Scientific System Reagents

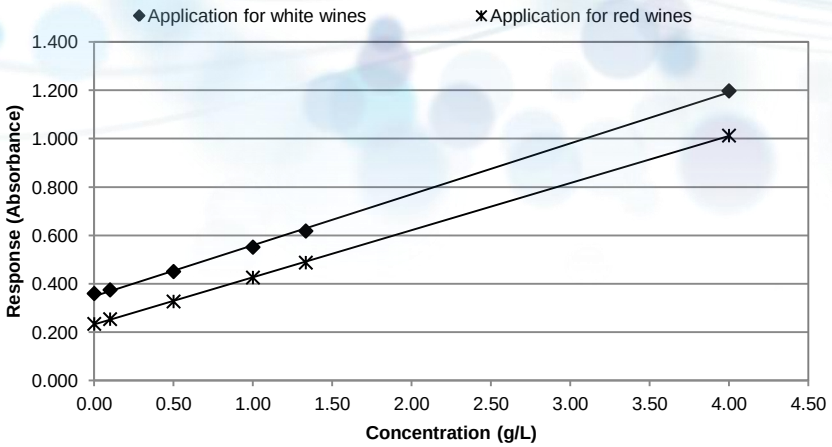
- Optimized system solution
  - System applications
  - Optimized kit sizes and on-board stability
  - Wide range of standards

- Productivity and efficiency
  - Ready-to-use liquid reagents eliminate reagent preparation
  - Minimal reagent waste
  - Bar-coded reagent vials provide easy and reliable identification
    - lot, expiration date, vial size
    - real-time reagent monitoring

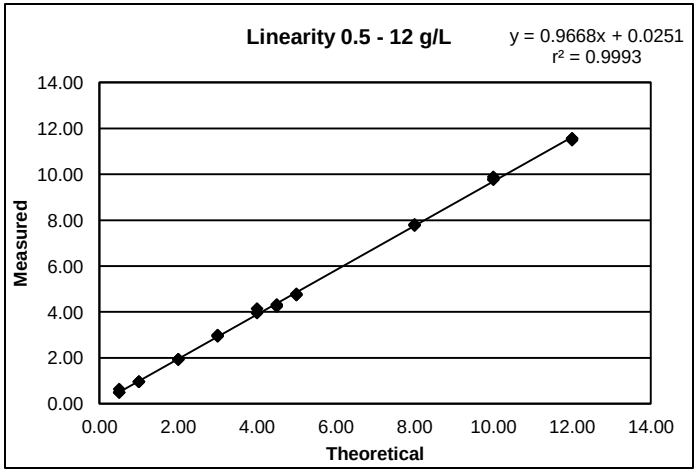
Example: Tartaric Acid Analysis from Wine

	White wine		Red wine	
	N	30	**N**	30
	Mean	2.76	**Mean**	2.11
	SD	**CV %**	**SD**	**CV %**
Within run	0.045	1.6 %	0.052	2.5 %
Between run	0.043	1.5 %	0.042	2.0 %
Total	0.062	2.2 %	0.067	3.2 %

- Precision CV 2 - 3%
- Measurement range from 0.5 mg/L to 12 g/L



- Calibration curves for white and red wines



- Linearity

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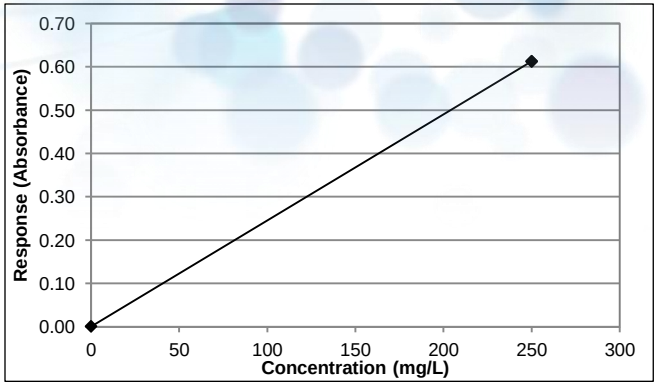
Example: L-Ascorbic Acid Analysis from Juice

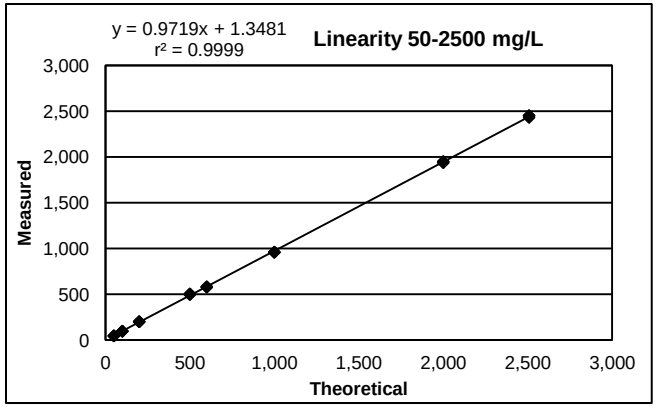
	Juice, orange (mean 118 mg/L)		Juice, raspberry, blueberry (mean 496 mg/L)	
	N	30	**N**	30
	SD	**CV%**	**SD**	**CV%**
Within run	1.014	0.9%	4.08	0.8%
Between run	0.523	0.4%	0.836	0.2%
Total	1.141	1.0%	4.164	0.8%

- Precision CV <1%

- Measurement range from 50 mg/L to 2500 mg/L



- Calibration curve



- Linearity

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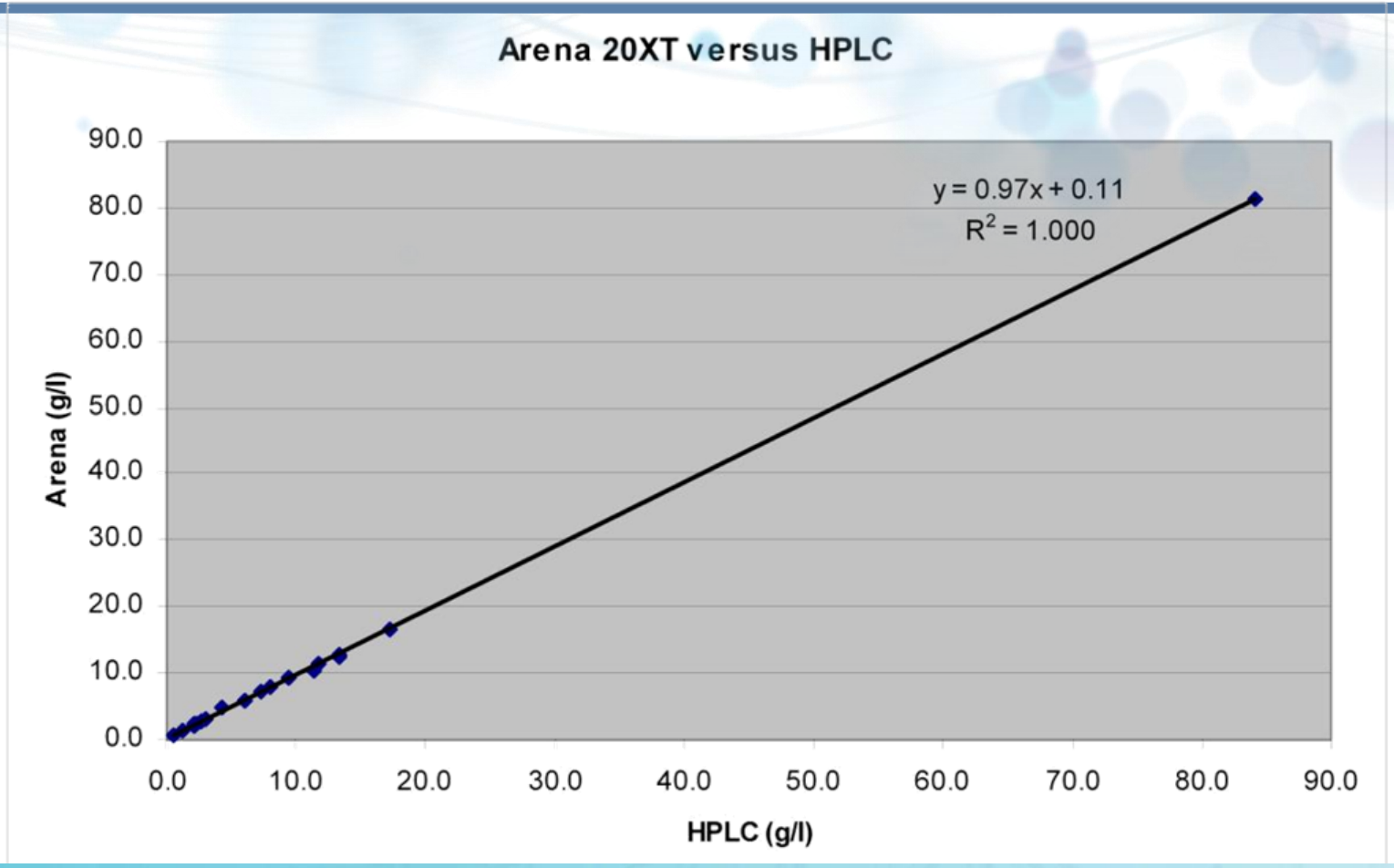
Performance of Sugar Analysis

For sugar analysis	Measuring range (g/L)	Precision CV%
D-Fructose	0.02 – 140	1.0 - 1.4
D-Glucose	0.02 – 140	1.6 – 1.7
D-Glucose + D-Fructose	0.04 – 200	1.0 - 1.4
D-Glucose + D-Fructose + Sucrose	0.24 – 200	1.6 - 2.7

- Wide measurement range with automated dilutions

Example: Method Comparison Study for Glucose



Evaluation of a Fully Automated Arena Assay for Measuring D-Glucose in Wines

Klemm, M. (1), Kaski, L. (1), Suoniemi-Kähärä, A. (1) and Lehtonen, P. (2)

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(2) Alcohol Control Laboratory, Alko Inc., P.O.Box 33, 00181 Helsinki, Finland

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DA Environmental Applications

- Chloride
- Fluoride
- Nitrate Hydrazine
- Nitrate Vanadium
- Nitrate Enzymatic
- Nitrite
- Total N (TON)
- Orthophosphate
- Total P
- TKN as N
- Total CN
- Total Hardness
- Sulfate
- Chromium VI
- Calcium
- Magnesium
- Silica
- Iron (ferrous)
- Ammonia
- Urea (ammonia)
- pH/conductivity
- Alkalinity

Reasons to Perform Wastewater Analysis

- Monitoring discharge
  - Regulatory limits
- Nutrient Analysis
  - Excessive plant growth in aqueous environments
- Known samples
  - Historical analysis
    - e.g., high chloride levels detected from a treatment facility with a water inlet near the sea/estuary
- Unknown samples
  - Investigative, pollution incident, farm run-off, milk spill, or industrial discharge due to plant failure

Common Anions in Wastewater

- Inorganic anions
  - Chloride
    - Disrupts nitrification process (treatment)
  - Sulfate
    - Disrupts anaerobic digestion process (treatment)
  - Phosphate, nitrate, nitrite
    - Plant nutrients; phytoplankton blooms
  - Bromide
    - Ozonation, chlorination -> Disinfection by-products: brominated trihalomethanes, bromate (carcinogens)
- Organic acids
  - Formic, acetic, propionic acids
    - pH balance

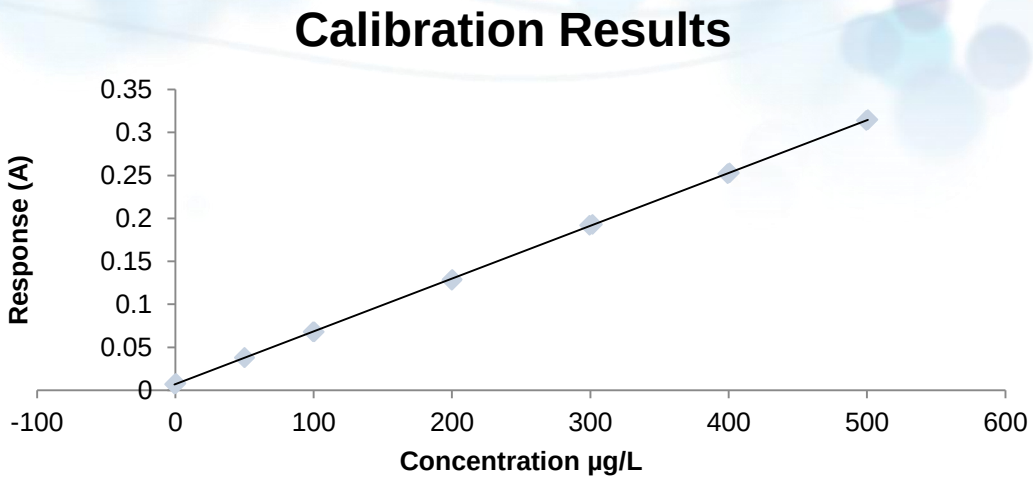
Anion Determinations Using Photometric Assays

- Manual wet chemistry assays
  - Labor intensive
  - Waste reagents
  - Error prone
- Continuous flow analyzers
  - Relatively slow
  - Generates a lot of waste
- Discrete analyzers
  - Rapid, automated, efficient

NEW Nitrate Enzymatic Assay

- Nitrate- nitrite enzymatic method
  - Provides highly specific measurements
- EPA approval for wastewater analysis in process (353.X)
  - Enzymatic Reduction Method for method 4500-NO_3-Nitrogen (Nitrate)
- A rapid, non-toxic alternative
  - Sample preparation is simplified
  - Detection range is flexible
  - Reduce costs in reagent usage and waste disposal

TON enzymatic Data



Calibrator	Response (A)	Calculated Concentration µg/L	Concentration
S0	0.007	-0.566	0
S0	0.008	0.497	0
S1	0.038	50.077	50
S1	0.038	49.926	50
S2	0.068	100.43	100
S2	0.068	99.548	100
S3	0.129	200.161	200
S3	0.128	199.822	200
S4	0.193	301.529	300
S4	0.192	299.386	300
S5	0.252	399.241	400
S5	0.253	400.542	400
S6	0.314	499.425	500
S6	0.315	500.628	500

International Standards Using Discrete Analysis

Chemical or Contaminant	ISO	EPA Method	SM	Description
Ammonium	15923-1	350.1	4500 NH3-H	Automated spectrophotometric determination with a discrete analysis system
Chloride	15923-1	325.2	4500 Cl-E	Automated spectrophotometric determination with a discrete analysis system
Nitrate	15923-1		4500 NO3-H	Automated spectrophotometric determination with a discrete analysis system
Nitrite	15923-1	354.1	4500 NO2-B	Automated spectrophotometric determination with a discrete analysis system
Phosphate	15923-1	365.1	4500 PE	Automated spectrophotometric determination with a discrete analysis system
Silicate	15923-1	370.1	4500 SiO2-D	Automated spectrophotometric determination with a discrete analysis system
Sulfate	15923-1	375.4	4500 $SO4^{2-}$ E	Automated spectrophotometric determination with a discrete analysis system
Chromium (VI)	11083	7196-A	3500-Cr B	Standard Methods for The Examination of Water and Waste Water
Fluoride		340.3	4500-F E	Standard Methods for The Examination of Water and Waste Water
Iron (Ferrous)	6332-1988		3500-Fe B	Standard Methods for The Examination of Water and Waste Water
Total Hardness		130.1	2340 C	Standard Methods for The Examination of Water and Waste Water
Alkalinity				Bromophenol blue method
Calcium		215.2		Arsenazo III Method
Magnesium				Xylidyl Blue I Method
Urea				Enzymatic urease method
Conductivity		120.1		Electrochemical method
pH		9040C		Electrochemical method

Discrete Analysis Routine Workflow

1.

Check/ run calibration

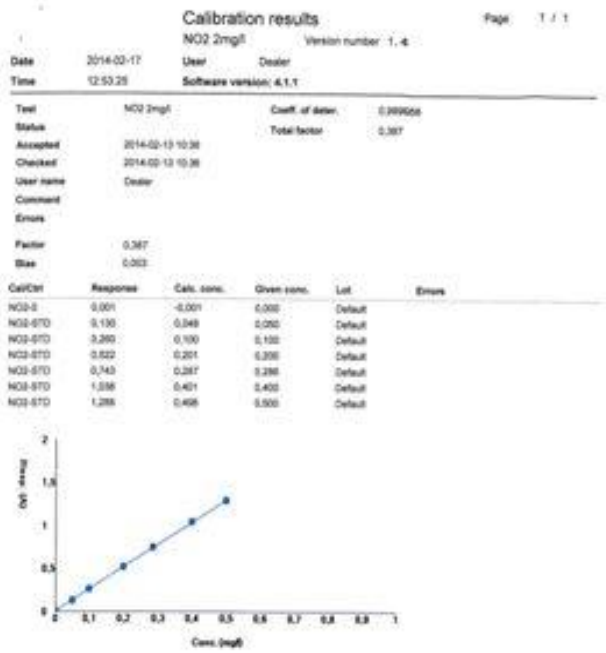
2.

Run samples:

- up to 54 at a time* with Gallery Plus
- up to 45 at a time* with Gallery

* continuous loading

3. Results


Calibration results

NO2 2mg/l

Version number: 1.4

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Time	12:53:25	Software version: 4.1.1	

Test	NO2 2mg/l	Coeff. of deter.	0.999958
Status		Total factor	0.387
Accepted	2014-02-13 10:36		
Checked	2014-02-13 10:36		
User name	Dealer		
Comment			
Errors			
Factor	0.387		
Bias	0.003		

Cal/Ctrl	Response	Calc. conc.	Given conc.	Lot	Errors
NO2-0	0,001	-0,001	0,000	Default	
NO2-STD	0,130	0,049	0,050	Default	
NO2-STD	0,260	0,100	0,100	Default	
NO2-STD	0,522	0,201	0,200	Default	
NO2-STD	0,743	0,287	0,286	Default	
NO2-STD	1,036	0,401	0,400	Default	
NO2-STD	1,288	0,498	0,500	Default	

Time to first results typically 10 min

Example Work-Flow

- Industrial Food Process Line
  - Requires analysis of phosphate and sucrose every 10 minutes
  - Tests can be performed immediately upon line start-up
  - Samples can be inserted as needed to confirm values
- Environmental Test Lab
  - Daily analysis consists of 30 nitrate, 30 chloride, and 10 Hexavalent Chromium (non-trace)
  - Estimated time to complete: 28 minutes
- Pharmaceutical QC
  - Requires analysis of glycerol and acetaldehyde on all finished lots
  - Complete tests as lot is finished, or in process
  - Time to complete 100 Glycerol tests: 44 minutes, first in 12 minutes
  - Time to complete 100 Acetaldehyde tests: 38 minutes, first in 10 minutes

Summary

- Discrete analysis is a fast and specific way to analyze a broad variety of analytes
- Utilizes colorimetric and enzymatic testing, as well as pH and conductivity
- Full automation for any photometric technique

Automated discrete analysis offers speed, flexibility, and reliability

Thank You!

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The world leader in serving science

Committed to our customers' goals
for better results and greater productivity