UV/Vis Spectroscopy:

Water Analysis
Choosing the best UV/Vis System

Water analysis for the environment or industry

Chris Lynch
July 2014
Safety of our drinking water supply is increasingly important in light of outsourcing and Homeland Security concerns.

Compliance with increasingly challenging regulations.

As the world population reaches toward 12 billion in the next 50 years*, greater pressures will be placed on arable land, water, energy, and biological resources.

Critical that wastewater meets required standards before release.

Instruments are used to measure quality, nutrition, compliance with labeling requirements, possible contaminants, and material properties.
The need for Water Analysis

- **Drinking Water**
  - Fresh water is becoming difficult to maintain in some parts of the world
  - How do you know if it is safe
  - What byproducts maybe affecting the quality of it?

- **Waste Water**
  - Industrial byproducts need to be contained
  - Protection of the environment is now critical

- **Process Water**
  - Water quality is critical to the manufacturing process worldwide
  - From manufacturing food to steel water is a major component of the process
  - Standards need to be maintained to protect product quality

- **Protection of the Ecosystem**
  - Discharge water must meet the standards or the damage to the Ecosystems are at risk
  - What about Nanoparticles in water, regulations will come
What does UV/Vis Technology offer?

- Simple inexpensive & accurate analysis
  - Wide dynamic range
  - Easy to use
  - Robust
  - And a lot of companies make them!

- Need more sensitivity, no problem
  - Simply increase the pathlength of cuvette

- Wide range of analysis
  - Inorganic
  - Organic
  - Biological
  - Clarity
  - Tribitity
Many different types of UV/VIS system are available today

➤ VIS, UV/Vis
➤ Single beam, single beam / split with reference channel / reverse optic
➤ Double beam
➤ What is the critical information you need to know when selecting the instrument?
  - Wavelength range
    - Does it cover the wavelength range I expect to need
  - Absorbance range
    - Will the instrument be capable of measuring over the absorbance range I need?
  - Stray light
    - This will have one of the biggest impact on your measurements
UV/Vis spectroscopy  the versatile technology every lab needs

- UV/Vis is one of the oldest and most common techniques found in most laboratories today
- Sampling flexibility, easy of use and cost make a powerful addition to any lab bench
- In general all UV/Vis instruments contain three major components
  - A source of polychromatic light
    - Tungsten-Halogen and Deuterium lamps
    - Single Xeon flash lamp
  - An optical component to separate the polychromatic light into the individual components
    - Monochromatic or single wavelength light
  - A detector to sense the energy after it has interacted with the sample
    - Photo Diode
    - Diode array
    - CCD
There are several common configurations of UV/Vis instruments

- **Diode Array**
  - Immune to external light, Reverse Optic design
  - Very fast, acquires full spectrum in a single scan
  - Typically higher Stray Light levels
    - Limited Dynamic range

- Generally lower cost
Types of Common Optical benches - Double beam systems

- Double Beam Spectrometer configuration
  - Overall best long term stability and reproducibility
  - Generally better stray light performance
  - Offer variable resolution
  - Support a wide range of path length's
  - Typically support more sampling options

- So why is this important to you?
  - Long term stability / Drift
    - Less time running baselines and more time running samples
    - Improved reproducibility
  - The better the basic performance of the instrument the wider the range of samples it will support.
Sampling flexibility is key in optimizing lab resources

- Single cuvette - Multi cuvette: How much automation should there be?
- 1cm to 10cm pathlength cuvettes: What is the difference?
  - Need to understand the effect of pathlength on sensitivity
  - Beer’s law: Why is this important?
- Autosampler’s - Save time and frees up valuable lab resources
- Be sure what you purchase has the flexibility you may need

Flexibility in cuvette selection

Time saving cell changers

Sipper pumps for Autosampler integration
Reference Materials provide performance validation

Reference materials are critical to any lab performing Routine testing

B2500099 Stray Light Solutions

B0507805 Photometric and Wavelength Accuracy filters

B2500100 Pharmacopoeia solutions
Where Would We Be Without Clean Water?

- Drinking water is one of the most overlooked commodities in America.
- Water is available everywhere the tap, drinking fountain, in our homes.
  - You can even pay premium prices for it in a bottle but it is always available.
- Now imagine it's not.
- Imagine a natural or worse, a man made disaster disrupts the supply.
  - Many of our citizens know first hand.
    - Is the water supply safe?
    - Can we have confidence in the data being reported?
    - Will it ever be the same?
- These are all issues for the government and every municipality in the country.
A Critical Situation for Many Municipalities

- Current infrastructure across the country needs updating
- EPA currently estimates more than $500 Billion will need to be spent over the next 20+ years
  - Distribution systems
  - Pipelines
  - Instrumentation
- Many municipalities are looking to the private sector for help
  - Many have outsourced their water supply needs
  - Many corporations across the country provide services
- The importance of tractability in data collection and analysis is now more important than ever
  - Validation of methods
  - Storage of electronic data needs to be protected
Public Safety Is Now of Paramount Concern

Accountability is Key

- Many companies provide chemistries to satisfy EPA requirements and reduce the possibilities of sample preparation errors
- Stable, highly repeatable UV systems are a key component
- Acquisition and storage of data is more important than ever
More cities are outsourcing analysis and processing needs to control cost
- The population however is going to look to the local government for answers during an event not the contractor!

Who oversees the contractors to protect the public interest?

If a problem develops how quickly can the necessary data be evaluated to determine the cause and corrective action?

Performance specifications are more important now than ever before. The need for long term stability trends is increasing as cities grow.
UV/Vis spectroscopy is an important analytical technique used for the determination of many water constituents.

Environmental regulations in many countries prescribe the use of UV/Vis spectroscopy. Depending on the method, UV/Vis determinations of metal and organic nonmetal analyses in water have a minimum detectability in the ppb-ppm range.

A large number of analytes can be measured with the same basic system. Only the chemistry changes.

Sample preparation, required chemicals and standard solutions, sensitivities, and interferences are well documented in common environmental handbooks.
A total of 60 example common water and wastewater environmental example methods based on US EPA and/or US Standard Methods guidelines are available for the PerkinElmer LAMBDA 25/35/45 operating with UVWinLab Version 5.1.5 or higher.

Methods can be imported into existing UVWinlab installations for routine use. In addition to the method file, a custom report template is provided for each analyte.

Protocols for each analyte are included, which were developed on the LAMBDA spectrometers. Complete documentation is available in the handbook “Water and Environmental Analysis” according to US EPA methods.

The availability of preprogrammed environmental methods eliminates the end user from having to “program” these methods, and ensures rapid implementation of these systems in water quality laboratories.

- User must verify and update as needed any method used to insure latest revisions and limits are used.
Control and Archiving of Electronic Data Will become Important

- Driven by the FDA in the Pharmaceutical industry it is likely other agencies will require more stringent control of data.

- This is critical should events occur or a long term trend begins to surface.

- Without an enhanced security software environment, the integrity of results from water quality laboratories can be in question.

- Archiving of data in protected databases will be needed in the future.
UV WinLab Enhanced Security Software Platform

Windows Explorer Look and Feel

Electronic Signature Provides Traceability
Method setup and Sample Information are AlwaysStored

Detailed sample information can be stored along with the data so it can always be accessed

Instrument setup parameters are protected once Method is approved
Instrument Performance Verification Capability is Included
UV WinLab - Database Querying and Trending
A Safe water Supply is Everybody's Concern

- Water is one of our most critical global resources and needs to be protected
- The analysis of it requires the right instrument and chemistries to do the job
- Importance of instrument, data integrity and traceability are now more important than ever before
Thank You

Questions ?