Water Quality Data at High Time and Space Resolution in the Field : Expanding Spectrophotometer Capabilities with Arduino Driven Sequential Autosampler

Bryan Maxwell, François Birgand, Kyle Aveni-Deforge and Brad Smith

Need for both high spatial and temporal resolution

- Biological and chemical processes often exhibit high spatial and temporal heterogeneity
- Data acquisition in environmental sciences is always partial in time and in space
- 'Hot spots' and 'hot moments' are thought to have a disproportionate impact on biogeochemical cycles
- There is demand for tools able to capture hot spots and hot moments *together* in the field (Fig.1)
- New UV-Vis spectrometer probes make high temporal resolution water quality measurements possible for many parameters

Research Questions

- Can a single high-frequency UV-vis spectrophotometer be fitted with an autosampler to measure multiple sources of water?
- Can the volume per sample be minimized to expand use for porous media systems?
- Can such a system provide sufficient precision to address new time-space resolution demands?
- What would be the performance and applications of such a system ?

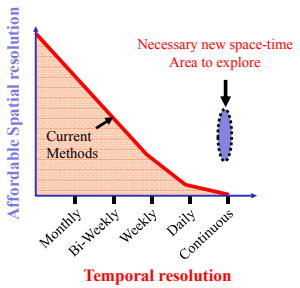
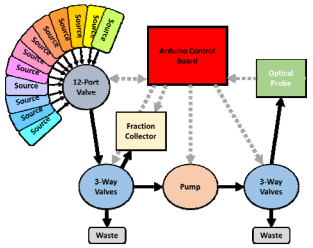
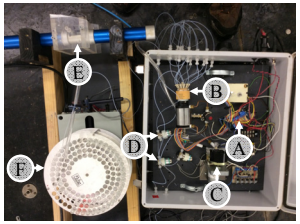


Fig. 1. Conceptual relationship between spatial and temporal resolution scales for current and desirable investigation methods in water quality and biogeochemistry

System Design and Functioning

- **Small sample volume:** less than 15 ml thanks to low volume cuvette and 0.9 mm ID PTFE tubing
- **Multi-port intake:** 12-way valve allows 12 different intakes from separate sources up to 12 m away
- **Several automated configurations** for pumping, purging and rinsing
- **Time resolution** per source better than 1 hour for each of the 12 sources
- **Arduino controlled** fully automated; works on 12V DC
- **Affordable sampler**: less than $5,000 to build
- **UV-vis spectrometer** : gives immediate, and rich data stream which can be analyzed to provides accurate results at high sampling frequency.
- **Fraction volume collector** : collects samples for lab analysis to calibrate/validate spectrometer results





Video of the system At work

Fig. 2. Top: flow chart of system. Bottom: An Arduino control chip (A) controls selection of the 12-way valve port (B), the pump (C) and 3-way valves (D) to control sampling configuration to s::can spectrometer (E) to fractional volume collector (F) for lab comparison.

Sample Routing Configurations

- System can be configured to minimize cross-contamination
- Several internal paths are available for
  - pumping,
  - rinsing
  - purging back to source or not
  - Volume collecting
- From source to probe and back to source (A & D)
- Rinsing cycle with DI water (C & F)
- Purging previously filled line (B) can occur before sampling to probe (A)
- Purging the manifold without sending back water to source (F)
- Automatic sampling to fraction collector (E). Pump is reversed to purge the fraction collector line with air (not shown) and the left over is sent to waste (F)

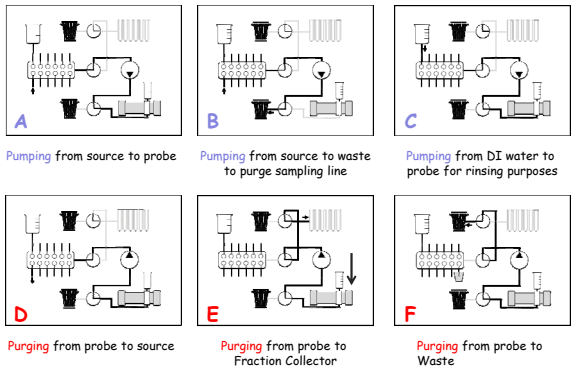


Fig. 3: Schematics of the different configurations available for pumping, purging, rinsing and sampling

System evaluation

- Surface tension causes small water droplets to remain in 0.9 mm diameter tubing
- → Potential for cross contamination
- Test system for riskiest configuration sequence, i.e. in Fig.3 ADCF, ADCF, etc. alternating sampling from two, low and high concentrations, bottles of 500 mL each
- Results show cross-contamination of less than 80 µL between consecutive samples (Fig. 5)
- It would take 2,500 samples to dilute 20L of water with DI water from 5.00 to 4.95 mg N/L of nitrate, i.e. ~ 7 days

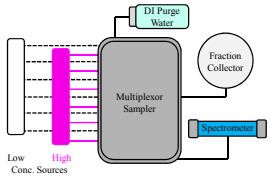


Fig.4: Alternating between low and high concentration sources to evaluate cross-contamination

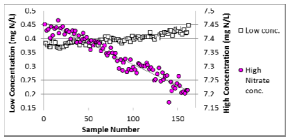
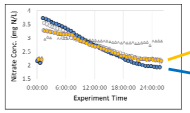
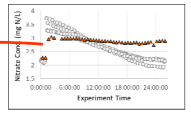


Fig.5: Changes in concentration in the two sources over time allows calculating apparent contaminating volume

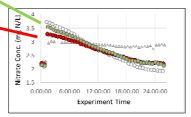
Application: in stream mesocosm study with replication

- 6 min per sample
- 36 min resolution for each mesocosm
- Allows refined kinetics calculations





Control



Conclusion

- Mini-volume automatic analyzer opens the possibility to explore new time-space resolution domain
- Low Cross-contamination warrants use of instrument in most situations
- Promising method for studying 'hot spots' and 'hot moments'
- Please visit our lab: