Data quality matters for biotic ligand modeling work: pH and DOC

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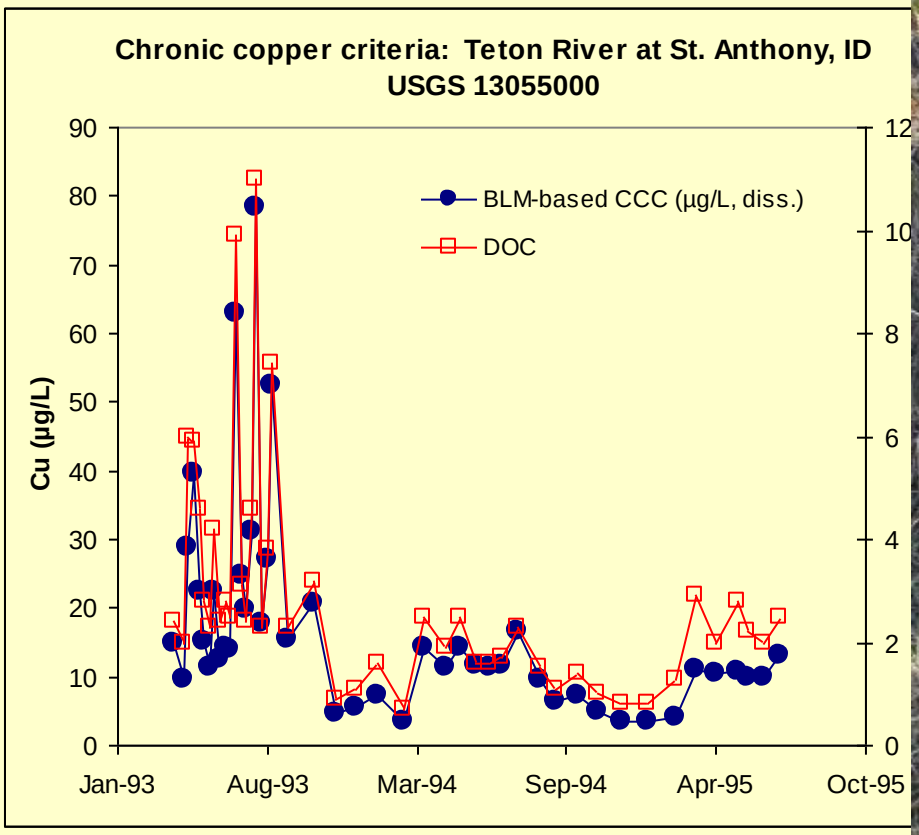
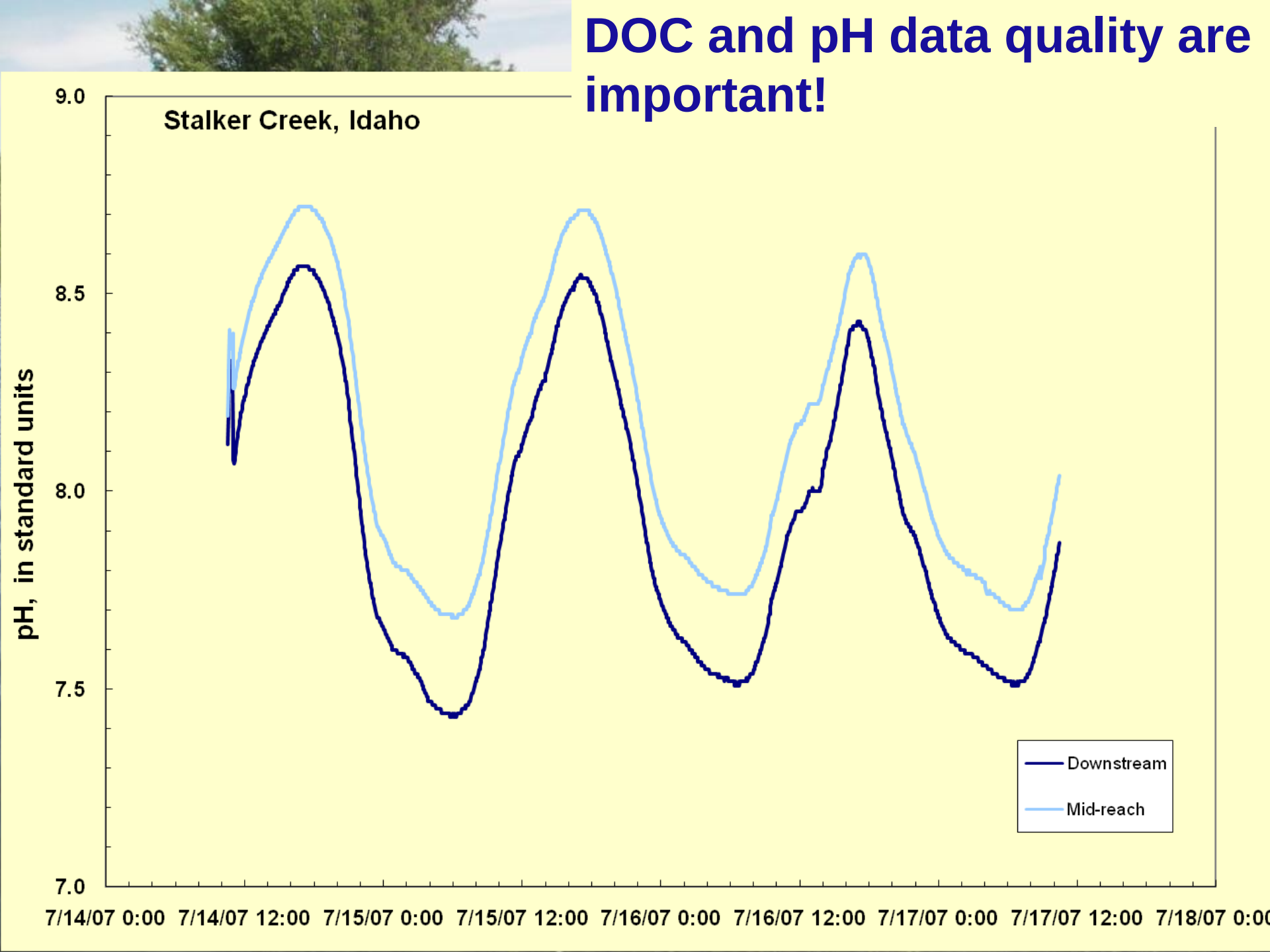
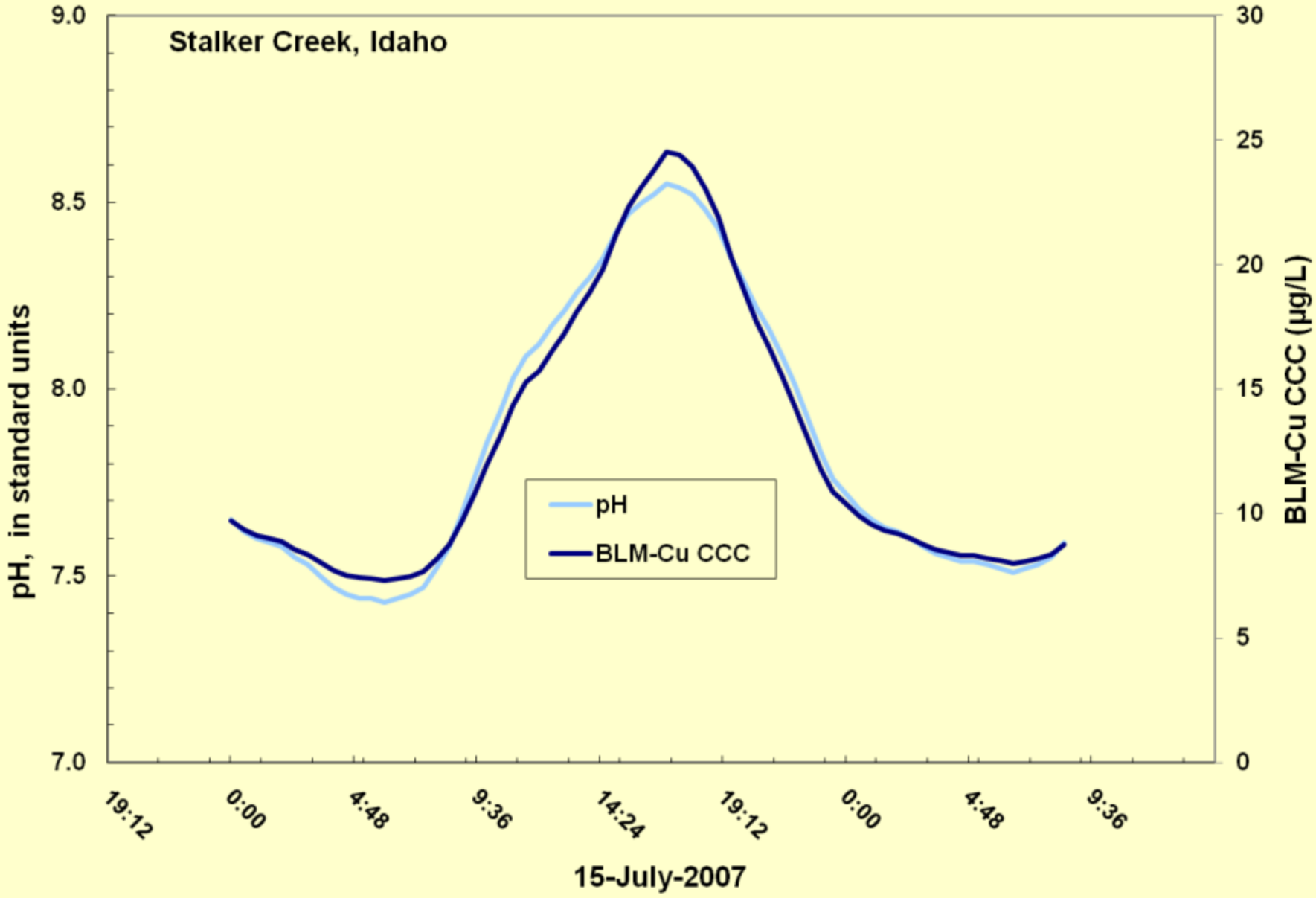
All analyses and data summaries shown in this talk are provisional and subject to revision

DOC and pH data quality are important!



DOC and pH data quality are important!




Stalker Creek, Idaho
pH, in standard units
BLM-Cu CCC (µg/L)
9.0
8.5
8.0
7.5
7.0
30
25
20
15
10
5
0
pH
BLM-Cu CCC
19:12
0:00
4:48
9:36
14:24
19:12
0:00
4:48
9:36
15-July-2007

USGS

pH

- Sampling early in the morning could give lowest (stringent) criteria; sampling in late afternoon could give highest (lenient) criteria
- What's most appropriate? Average? Lowest?
- Natural daily cycles and criteria implications are largest on low gradient, productive streams. Much less of a concern in small, high gradient mountain streams
  - Silver Bow Creek near Butte, MT – 2 pH units
  - Silver Creek Idaho – 1 pH unit
  - 8 agricultural streams in S. Idaho – 0.5 to 1 unit
  - Panther Creek, Idaho – 0.6 units
  - Big Deer Cr (trib to Panther) – 0.1 units
  - 5 streams near Stibnite, ID – 0.1 to 0.2 units
- Proper calibration and meter operation obviously important
- At fixed sites (e.g., downstream of a permitted outfall) a continuously recording meter would be beneficial

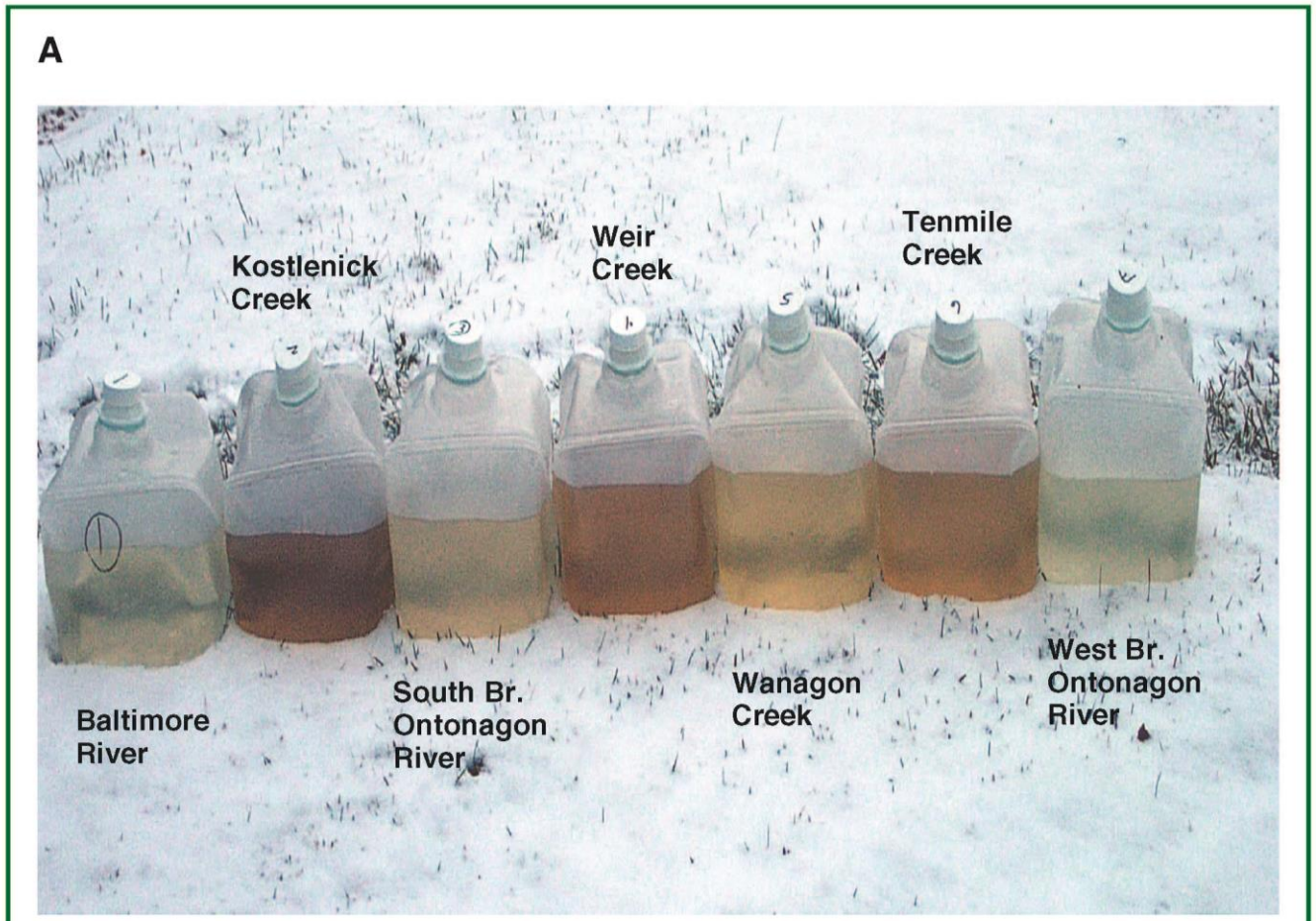
USGS

pH

Best Practices?

- **Proper calibration and meter operation obviously important**
- **At fixed sites (e.g., downstream of a permitted outfall) a continuously recording meter to capture daily cycles would be beneficial**
- **Otherwise make some adjustment to account for likely daily cycles? In absence of cycle data, assume a pH value of 7?**

Dissolved organic carbon (DOC

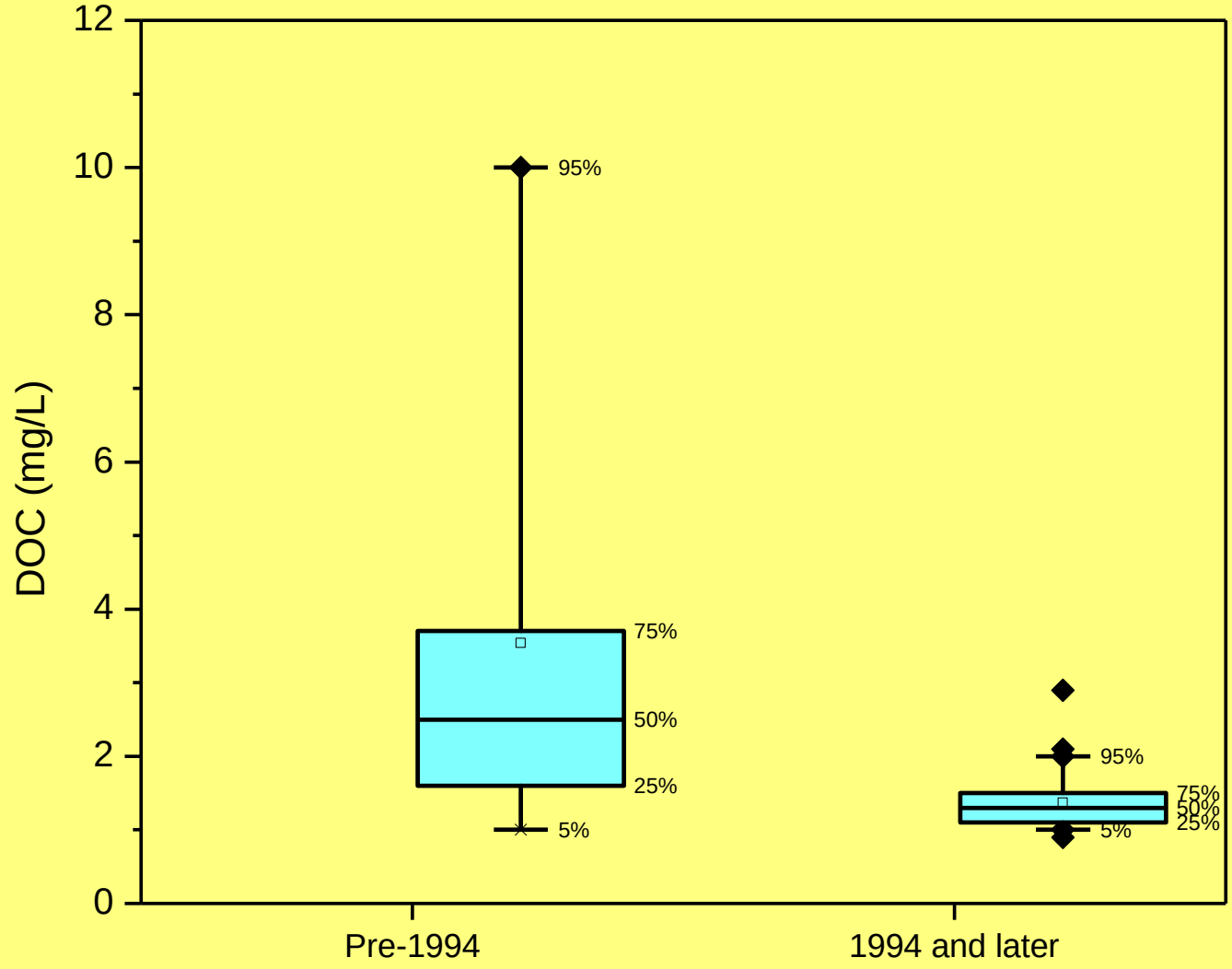


Natural DOC in stream water may be highly variable and protects against copper toxicity

Findlay, S. E. G. 2006. Dissolved organic matter. p.240 *in F. R. Hauer, and G. A. Lamberti, editors. Methods in Stream Ecology, Second Edition. Academic Press (Elsevier). Used by permission of Elsevier*

For example, beware of USGS DOC data prior to 1994!

Columbia River between Northport, WA and Trail, BC



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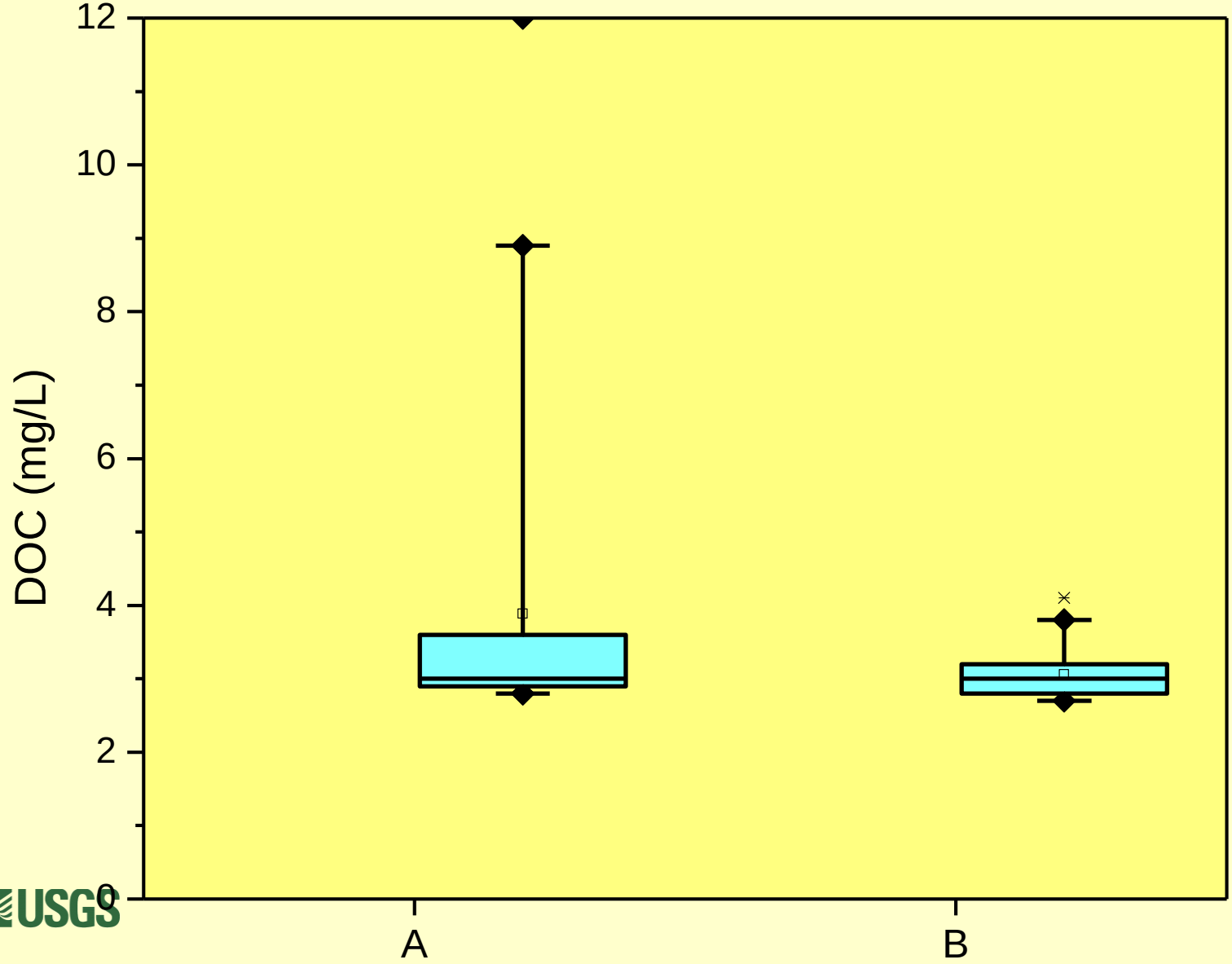
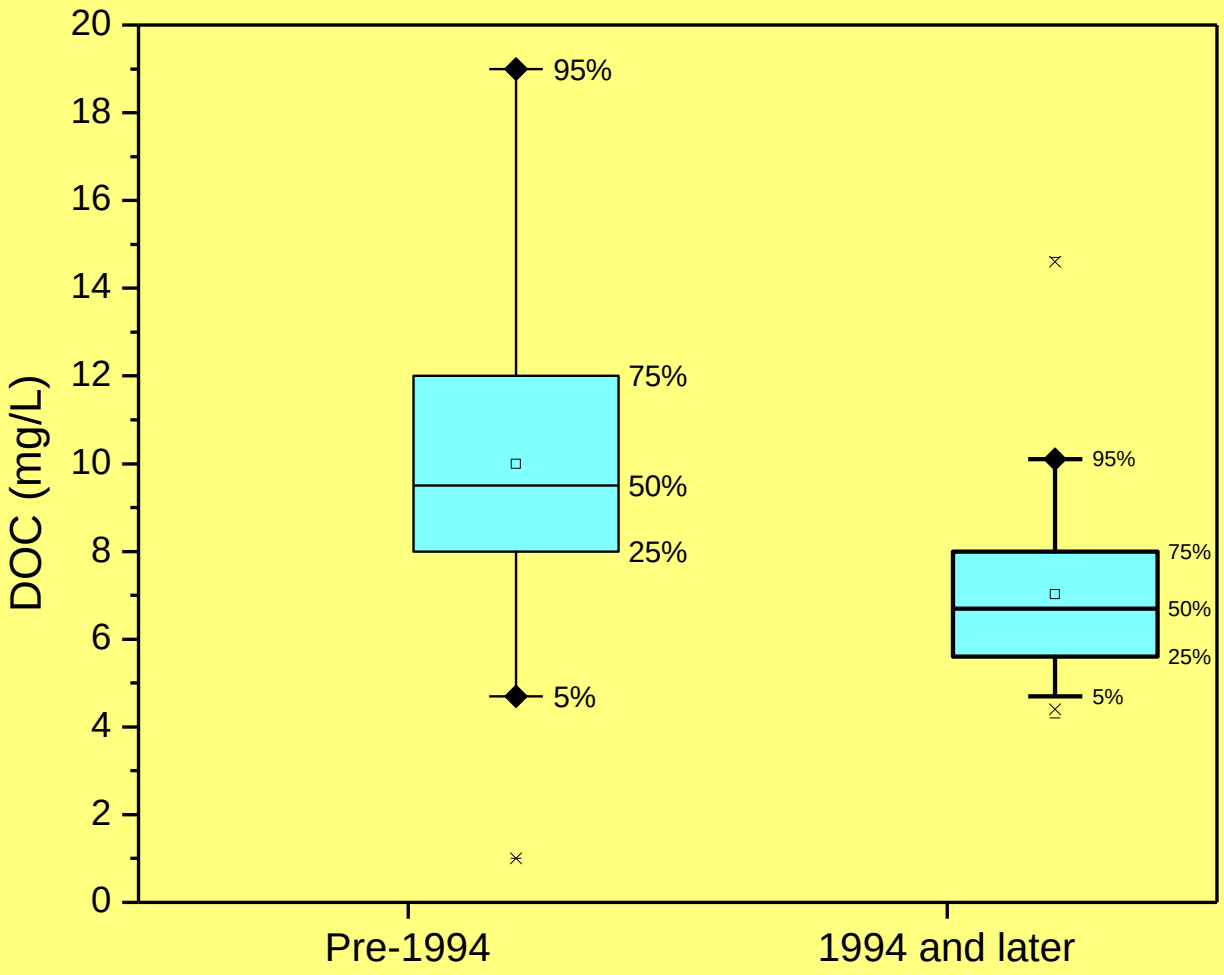
Colorado River downstream of Glen Canyon Dam, Arizona



Neuse River, North Carolina coastal plain



Unnatural DOC sources can high bias samples

Contamination from filters and bottles are a widespread issue

OWQ WaQI Note

August 6, 2008

Office of Water Quality Water-Quality Information Note 2008.13

Subject: Field Methods—Discontinue use of Brand A capsule filters for dissolved organic carbon (DOC)

Brand A's particular model of capsule filters (name redacted) beginning with lot number 1873, are no longer to be used for filtering samples for analysis of dissolved organic carbon (DOC). Quality-assurance tests run by the Quality-Assurance Section at the National Water Quality Laboratory (NWQL) showed DOC levels between the long-term method detection level (LT-MDL) and the laboratory reporting level (LRL) after a 1-liter rinse. Levels of 18.2 and 21.1 mg/L of DOC were seen in the first 125 mL of the rinse water. Because DOC levels appear to be increasing in recent capsule filter lots, the decision has been made to discontinue the practice of using capsule filters for processing DOC samples.

In lieu of the Brand A capsule filters, the Brand B filters (name redacted) or the 25-mm baked, glass-fiber filter (Q441FLD) can be used for processing DOC samples. The 25-mm filter must be used with the Teflon DOC-25 filter unit (Q444FLD) or a filter funnel and flask (see National Field Manual (NFM) Ch. 5.2.2.C for equipment information and instructions [http://water.usgs.gov/owq/FieldManual/chapter5/pdf/chap5.pdf]. This Note modifies this section of the NFM.

Unnatural DOC sources can high bias samples

Issue probably better known in the oceanographic community than water quality monitoring community

Pergamon

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RESEARCH NOTE

DISSOLVED ORGANIC CARBON CONTAMINATION INDUCED BY FILTERS AND STORAGE BOTTLES

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(First received June 1998; accepted in revised form September 1998)

Abstract—To optimize experimental protocol for marine dissolved organic carbon (DOC) studies in laboratory conditions, we examined the potential DOC releases from filters of different qualities as well as those from different types of bottles during 10 day-storage of Milli-Q water and 0.2 μm-filtered seawater. The results showed that utilization of 47-mm circle filters including polycarbonate (0.2 and 1 μm-pore size), polytetrafluoroethylene (PTFE: 0.5 μm-pore size) and aluminum oxide (0.2 and 0.02 μm-pore size) may induce significant DOC contamination ranging from 12 to 42 μM C for the first hundred milliliters of the filtrated solutions. However, filtrations of 2 to 4 l of Milli-Q water decreased the DOC blank of the filters to 2–5 μM C. As expected, precombusted (450°C, 6 h) glass fiber filters rinsed with 0.5–3 l of Milli-Q water produced very low blanks (1–4 μM C). We found that 10 day-storage (15°C, in the dark) of Milli-Q water and 0.2 μm-filtered seawater (250 ml) into 1 l-polyethylene, polycarbonate and perfluoalkoxy (PFA)-Teflon bottles, initially cleaned with HCl 1% and abondantly rinsed with copious amounts of Milli-Q water as well as in precombusted glass bottles (450°C, 6 h) induced very low DOC contamination of the solutions (0–5 μM C). Although complete DOC-free contamination experiment is difficult to reach particularly in shipboard conditions, these results strongly

DOC

Best Practices?

- **Include field blanks in sample collection; adjust data by subtracting out the value from the blank water**
  - **Not a perfect solution: even blank water has trace DOC**
- **If samples can be quickly delivered to the analytical lab (eg chilled and overnighted or frozen), consider having the lab filter the samples instead of doing it in the field**

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