



Aquatic Calibration and Validation Activities and Future Needs

HPLC Uncertainties: A Case Study for Establishing Guidelines and Review Procedures for Essential Climate-Quality Data Record (CDR) Analyses

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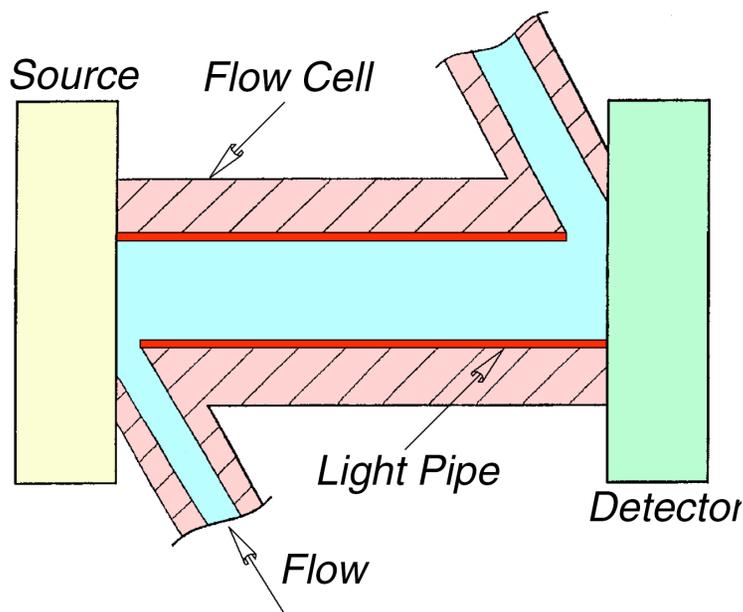
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**This and additional documents:
<http://oceancolor.gsfc.nasa.gov/DOCS>**

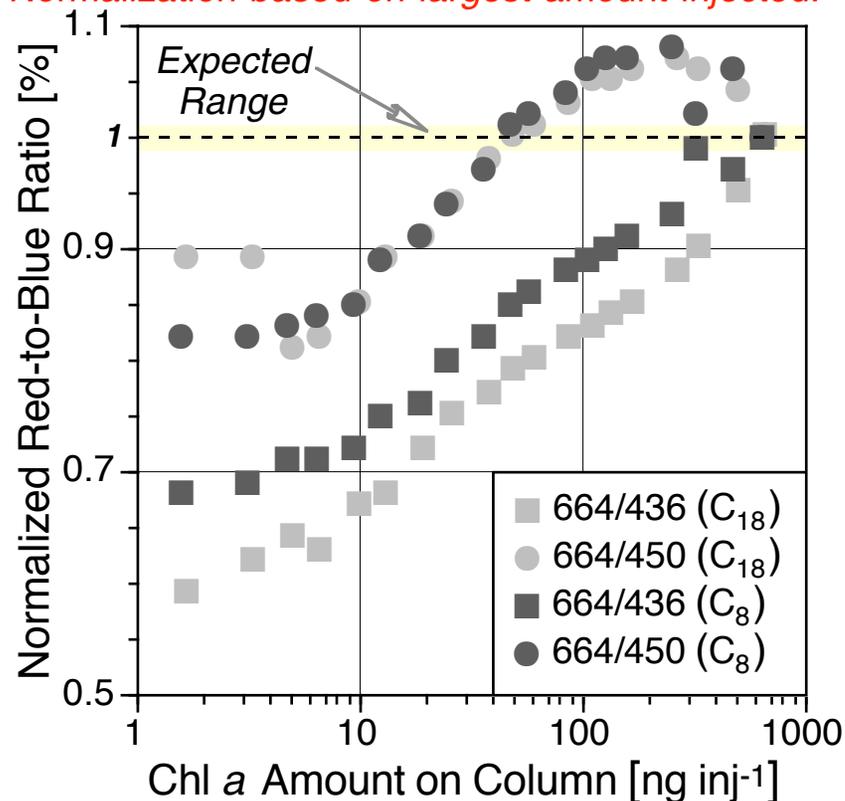


The Nonlinearity of the CHORS UV6000 Detector Invalidates All C₈ and C₁₈ Results (~24,000 Samples)

The UV6000 flow cell (US patent 5,608,517) uses a thin polymer (dark red) to pipe light down the flow cell with an optimal response in the ultraviolet domain (190–300 nm):



Normalization based on largest amount injected.



Nonlinearity is caused by two problems (US patent 6,281,975B): a) light can be piped inside the cell wall so it never sees the sample, but is seen at the detector, and b) light is reflected back into the flow path, but still spends some time in the cell wall not interacting with the sample. European patent 1,478,913C describes stray light issues from reflectance in the cell wall: the characteristics of the polymer makes the material more opaque at 200 nm than at 600 nm.



Options to Consider

The main difficulty with the CHORS data is each attempt to peel back a layer of the problem has exposed a new problem. Options for any future effort are as follows:

1. Classify the data as being unsuitable for calibration and validation activities, remove them from SeaBASS (already done), and do no additional work. In a few years many sampling holes will be filled by ongoing research and the HPL contract. Individual PIs would have to determine the applicability of existing CHORS data to their research objectives (past and present).
2. Attempt to characterize the nonlinearities for Chl *a* (the most extensively calibrated CHORS pigment and probably the most important), establish a correction scheme, and correct the data. This will require new resources and personnel (CHORS stops working on this problem 31 May 2008).
3. Attempt to characterize the nonlinearities for the primary pigments, establish a correction scheme, and correct the data. This will require substantial new resources (reintegration of some pigments is likely).
4. Attempt to characterize the nonlinearities for all the pigments CHORS reported, establish a correction scheme, and correct the data. This will require very significant new resources (reintegration of many pigments).
5. A final option—*suggested by more than one PI*— is to ignore the problem and leave the data as is.



Questions to Address

The questions for the Breakout II sessions encompassed more than the quantitation of HPLC pigments and included all the aspects associated with aquatic calibration and validation activities:

- *What does the carbon cycle and ecosystems community expect of this effort?*
 1. Round robins and workshops focused on understanding the sources of uncertainties are essential (including a recurring assessment and evolution of the protocols being used).
 2. Performance metrics need to be established for all analyses important to CDRs.
 3. All analyses for CDRs must have a quality-assurance plan (QAP) that is approved by the program manager or cognizant project office.
- *What are our biggest challenges in this area, and how do we address them?*
 1. Establishing calibration and validation capabilities for parameters other than Chl *a* and apparent optical properties (e.g., IOPs, DOC, DIC, etc.) will require a significant investment in time and resources.
 2. An oversight process with specific guidelines (at the program or project office level) is needed to a) ensure inspections and compliance with the QAP, and b) strengthen the peer-review process.



Questions to Address (*cont.*)

- *Is our list of identified data records complete, or is something missing?*
 1. Future science questions associated with the coastal ocean and near-shore processes are going to require a greater diversity of data products than are being produced now. Many of the measurements involved do not have calibration standards, so the calibration and validation of many future data products is going to require an investment in establishing certified reference materials and traceability.
 2. The ensuing data products should be archived in or linked with SeaBASS (especially metadata), because it is a unique repository of calibration and validation data.
- *Does the carbon cycle and ecosystems community need to establish priorities for these and other activities, and, if so, how should they be established?*
 1. It was recognized that limits need to be placed on the amount of data to be archived in SeaBASS, but a prioritization scheme was not agreed to.
 2. Everyone agreed the radiometric data need to be at the highest quality possible; the additional data products needed for interpreting near-shore imagery need to be prioritized at a similar level of data quality.