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10, C1168-C1170, 2013

Interactive Comment

Interactive comment on "Technical Note: Dissolved organic matter fluorescence – a finite mixture approach to deconvolve excitation-emission matrices" by A. Butturini and E. Ejarque

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General comments:

This technical note serves as an important and timely publication, as it addresses an area of research that is of interest to a wide range of parties. The authors clearly and succinctly describe the use of fluorescence spectroscopy for the characterization of dissolved organic matter, as well as the dependence of the meaningfulness of the data on the chosen method of interpretation. The authors mention existing statistical multi-

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variate methods of EEM interpretation, acknowledging their associated advancements in the use of fluorescence spectroscopy. Despite the widespread use of these methods, the authors address two main weaknesses of these existing EEM interpretation methods: the need for a large set of EEMs and the need for EEMs that follow some type of gradient, e.g., a salinity gradient.

In response to these weaknesses, the authors propose an alternative method for the evaluation of dissolved organic matter EEMs involving simple surface analysis and the finite distribution mixture approach. The main benefit of this model is its ability to evaluate an individual EEM without it coming from a much larger set of EEMs collected along a gradient. Although not mentioned in the technical note, this model, owning to its simplicity and "user friendly" nature, has the potential to greatly increase the usefulness of fluorescence spectroscopy for those monitoring dissolved organic matter in natural and engineered systems. For example, fluorescence measurements of influent water at a drinking water treatment facility for the purpose of predicting disinfection byproduct formation, chemical demand, and other downstream processes dependent on organic matter quality.

Specific comments:

Minor comments are listed below-

- 1. Introduction, page 4713, line 20: The authors state "A basic difference with respect to these tools lies in the assumption that peaks fit a predefined probabilistic density function". Can you increase the clarity of this sentence? More specifically, do existing multivariate tools make this assumption or is it the model proposed in this work that makes this assumption?
- 2. Do the authors assume that the 21 EEMs used in this study do not follow a gradient? The samples were collected "along the longitudinal continuum" of a river; is it assumed that the anthropogenic impact upon the river negates any longitudinal gradient?

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3. How does this model or the interpretation of results from this model address fluorescent components with multiple peaks? Previous work with PARAFAC and pure fluorescent substances have shown that one type or group of fluorophores is capable of exhibiting multiple peaks, however, this model appears to address each peak as its own independent group of fluorophores. The authors mention coexistence and correlation between peaks (in discussion and Table 3); does a certain level of correlation suggest that two peaks vary together because they are representative of the same group of fluorescent organic matter?

Technical corrections:

Minor technical suggestions are listed below-

- 1. Abstract, line 5: Replace "deconvolves single EEM" with "deconvolves individual EEMs"
- 2. Introduction, page 4713, line 10-13: Consider rewording this sentence, as it is a bit confusing and long winded. Consider something along the lines of "Conversely, to our knowledge, an algorithm that decomposes the signal of an individual EEM is currently unavailable. Such an algorithm would allow researchers to evaluate DOM quality using a reduced number of EEMs, as well as the freedom to compare and evaluate EEMs that do not necessarily follow any gradient".
- 3. Introduction, page 4713, line 19: Insert comma between "techniques" and "FDM"
- 4. Introduction, page 4713, line 22: Insert "a" between "necessarily" and "synonym"
- 5. Table 2: The title indicates twelve identified peaks, but the table and discussion only mention eleven peaks (P1-P11).

Interactive comment on Biogeosciences Discuss., 10, 4711, 2013.

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