The Importance of Validating Source Identification Results and Evaluating Alternative Hypotheses in a Forensic Evaluation

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Background/Objectives. Source identification and apportionment using receptor models is the backbone of many sediment forensic evaluations. To perform such an analysis, the researcher typically develops a hypothesis regarding potential sources, conducts the analysis, and based on the results accepts, rejects, or refines the hypothesis. If the results support the hypothesis, the results are often simply accepted as proof of the original hypothesis without additional evaluation. All too often the researcher does not conduct a sample by sample detailed analysis of the model fit but rather evaluates the model based solely on the overall goodness of fit. Furthermore, plausible alternative hypotheses are often left unstated and are not considered. These shortcuts can lead to erroneous conclusions and a flawed model of the sources and their contributions to sediment contamination. The objective of this paper is to define a systematic approach for both validation of the fit of the statistical models and the evaluation of alternative hypotheses in addition to the primary hypothesis.

Approach. We have developed a set of principles for validating source identification and apportionment receptor modeling results. At a minimum (1) assume that the model has flaws and seek to uncover and assess them before accepting the model; (2) conduct a detailed analysis of the overall model fit (3); conduct a detailed comparison of the source profiles derived by the model to a library of hypothetical source profiles (by analyte); (4) compare the contributions of individual analytes predicted by the model to the observed contributions for each analyte; and (5) for each sample, compare the predicted composition to the observed composition by calculating the sum of squares of the errors. If the model fit is judged to be sufficiently good, the next step is to use the model results to evaluate hypotheses regarding sources. For this analysis, it is critical to formally define the primary hypothesis as well as competing alternative hypotheses that might also explain the results. We demonstrate the influence of these factors using case studies.

Lessons Learned. The case studies demonstrate the value of formal validation of forensics receptor models. These procedures provide a powerful mechanism to identify possible errors in the model, even when the overall model fit, based on simple goodness of fit statistics such as R^2, suggest that the model is performing well. For example, sources that impact a small number samples or represent a minor component are easily missed without proper validation. These 'minor' contributors may prove critical in understanding sources and/or fate and transport. The evaluation of alternative hypotheses with the primary hypotheses can guard against making definitive assertions that may prove untrue. For example, during the preliminary review of the industrial history of the area, the researcher might identify a single potential facility as a match for the predominant source from the model, accepting the hypothesis that this facility is the sole source. However, if the researcher conducts a more detailed review of historical records for other source locations that match the profile, the alternative hypothesis that there are multiple sources can be evaluated. As with any scientific hypothesis, the evaluation of alternative hypotheses should be an integral part of any forensic evaluation.