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High performance size exclusion chromatography with a multiple wavelength absorbance detector for improved dissolved organic matter characterisation and water quality monitoring

Huiping Huang

School of Chemical Engineering

Faculty of Engineering, Computer and Mathematic Science

The University of Adelaide

Adelaide South Australia

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Abstract

This study was to develop better use of chromatographic data for dissolved organic matter (DOM) characterisation using data analytics approach. The findings confirmed that understanding the characteristic and composition of DOM was essential for water quality investigation and this task was highly demanding. Among different DOM analytical techniques, high performance size exclusion chromatography coupled with a photodiode array detector (multi-wavelength HPSEC) for multiple UV-Vis wavelengths measurement was proving to be a simple and informative choice of analytical technique for characterising DOM in the aquatic environments including drinking water supply systems. Compared to using single wavelength detection alone, the additional information imparted by multi-wavelength detection provided better understanding of DOM and yielded more insight into the key information that has more relevant in the field of water research. The development also solved some fundamental problems in multi-wavelength HPSEC analysis including multivariate chromatographic data exploration, resolution optimisation, and information extraction as well as applying the technique for further qualification and quantification of DOM in complex environmental and engineering aquatic samples.

In the early phase of this study, one of the aims was to access the suitability in using an open and free software program, R (version 3.1.0, R Development Core Team) to handle the complex chromatographic data. The data analytics procedures and program codes were developed in the direction of improving multi-wavelength HPSEC data exploration, interpretation and information extraction. This study also explored the applicability of this approach for DOM characterisation in water supply management. The benefits of this approach were demonstrated in two case studies. The case studies were carefully selected to bridge the knowledge gap of exploring the use of HPSEC as an environmental monitoring tool in a stormwater catchment and a drinking water distribution system. Both case studies shared a common aim of using HPSEC as a characterisation tool to determine the molecular profile of DOM and using the analytical information to understand the impact of DOM on 1) stormwater and 2) drinking water quality. Case study one demonstrated the proposed approach could provide better understanding the complexity of DOM in stormwater and the influences of environmental conditions (seasonal variations) and storm event characteristics (rainfall-runoff process) on stormwater DOM

characteristics. Case study two demonstrated the proposed approach could also provide better understanding of the association between DOM molecular weight distribution and nitrification occurrence in a chloraminated drinking water distribution system. Results confirmed the usefulness of multi-wavelength HPSEC analysis for providing additional knowledge of DOM characterisation and it can also allow the examination of changes to the molecule weight profiles in the lower wavelength region (below 254 nm). Correct selection of the UV wavelengths can be an important factor for providing appropriate indicators for water quality analysis. The detector wavelengths, 210 and 254 nm were found to provide useful information on the physiochemical properties of DOM in both stormwater and chloraminated drinking water distribution system. The ratio A_{210}/A_{254} could be used to estimate the proportions of functional groups and conjugated carbon species in the stormwater-associated DOM.

In addition, a package of simple analytical techniques, such as dissolved organic carbon (DOC), UV absorbance at 254 nm (UV_{254}), colour, turbidity, nitrate, nitrite, ammonia, total disinfectant residual and microbiological technique (flow cytometry) for bacterial level analysis were also selectively applied and their applicability to indicate water quality changes were evaluated. The correlations of water quality parameters derived from different methods were also statistically analysed using the R software. Pearson's Product Moment Correlation (PPMC) was used to evaluate the correlations among generate water quality parameters, HPSEC-UV profiles and microbiological analysis. The standard analysis of variance (ANOVA) was utilised to evaluate the significant influence of seasonal variation on DOM characteristics.

The findings of this research contributed to new knowledge in DOM characters and demonstrated the potential of using multiple water quality parameters combined with DOM characterisation tool for monitoring stormwater quality, understanding the performance of conventional treatment processes and the assessment of water quality in a water distribution system. This research also highlighted the useful application of chemometric approach provided by the R software program for improving HPSEC-UV analysis of DOM in aquatic systems. In addition, this development can lead to the inclusion of using multi-wavelength HPSEC as monitoring technique for the water quality management system

Declaration

I declare that this thesis presents work is carried out by myself. This work contains no materials which have been accepted for the award of any other degree or diploma in my name in any university or other tertiary institution; and to the best of my knowledge, contains no material previously published or written by another person, except where due references have been made in the text. Additionally, I certify that no part of this work will, in the future, be used in any university or other tertiary institution without the prior approval of The University of Adelaide and where applicable, any partner institution responsible for the joint award of this degree.

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All substantive contributions by others to the worked presented, including jointly authored publications, is clearly acknowledged.

Huiping (Ophelia) Huang

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