## T2R2 東京科学大学 リサーチリポジトリ Science Tokyo Research Repository

## 論文 / 著書情報 Article / Book Information

題目(和文)	
Title(English)	Elucidation and correction of fluorescence quenching for accurate prediction of chlorination by-products
著者(和文)	SaipetchKornravee
Author(English)	Kornravee Saipetch
出典(和文)	学位:博士(学術), 学位授与機関:東京工業大学, 報告番号:甲第11239号, 授与年月日:2019年6月30日, 学位の種別:課程博士, 審査員:吉村 千洋,鼎 信次郎,中村 隆志,藤井 学,朝倉 則行,越後 信哉
Citation(English)	Degree:Doctor (Academic), Conferring organization: Tokyo Institute of Technology, Report number:甲第11239号, Conferred date:2019/6/30, Degree Type:Course doctor, Examiner:,,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
 種別(和文)	論文要旨
Type(English)	Summary

## 論文要旨

THESIS SUMMARY

専攻: Department of	土木工学	専攻	申請学位(専攻分野): Academic Degree Requested	博士 Doctor of	(philosophy)	
学生氏名:	Kornravee SAI	PFTCH	指導教員(主):	吉村千洋		
Student's Name	Rormavec bhi		Academic Supervisor(main)			
			指導教員(副):			
			Academic Supervisor(sub)			

## 要旨(英文800語程度)

Thesis Summary (approx.800 English Words )

This thesis entitled "Elucidation and correction of fluorescence quenching for accurate prediction of chlorination by-products", which consists of seven chapters. Although, many predictive models for prediction of chlorination by-product are reported but the error of such models are still higher than the level of regulated concentration of chlorination by-products. Thus, an improvement of the prediction accuracy of models for chlorination by-product prediction is necessary. Fluorescence excitation-emission matrix (EEM) is believed as the best representative of the precursor of chlorination by-products due to the common aromatic structure with the precursor of chlorination by-product. Thus, EEM is often applied to indicate chlorination by-product precursor in natural organic matter (NOM) in an effort to obtain the greatest prediction accuracy. However, humic substances are known to quench fluorescence intensity of amino acids (AAs) and proteins. None of EEM-based models for chlorination by-product prediction explicitly integrate such quenching effect, although high percentage (around 35-52%) of intensity of amino acids fluorescence was quenched by the interaction with humic substances. Thus, the aim of this study is the improvement of an accuracy of models for prediction of trihalomethane concentrations (THMs) of the THM formation potential (THMFP) test by using EEM with correction of fluorescence quenching obtaining from elucidating of inter-component interaction of NOM. To this end, this study was done following the chapter 1 to 7 and the brief summary of the content in each chapter are listed below.

Chapter 1 is the introduction which describes the overall background, the importance of this study, summary of main contents and propose of this study

Chapter 2 is the literature review which explains about chlorination by-products and the current status on the application of fluorescence in the predictive model of chlorination by-product.

Chapter 3 is the investigation on the importance of correcting for fluorescence quenching in fluorescence based-prediction of THM in THMFP test of synthesis water samples from fluorescence titration between Suwanee NOM (SWNOM) and protein (Bovine serum albumin, BSA). Fluorescence quenching of BSA fluorescence was found to affect to the prediction accuracy of the models for chlorination by-products prediction and the correction of fluorescence quenching is necessary for the improvement of the prediction accuracy. The models using corrected (unquenched) fluorescence intensity exhibited the highest model fitness among models using other type of water quality parameters as indicator of THM precursors (e.g., dissolved organic carbon, DOC).

Chapter 4 is the investigation of the mechanism of an inter-components interaction in dissolved organic matter by using multi-spectroscopies. From fluorescence titration, static quenching is the type of fluorescence quenching of BSA by SWNOM which implies binding interaction between them. The interaction between SWNOM and protein (Bovine serum albumin, BSA) is found to have the effect on the H-boding of the secondary structure of the BSA, which leads the BSA conformational change and loss of its fluorescence intensity.

Chapter 5 is the generation of the empirical equation for correction of fluorescence quenching of BSA fluorescence by the interaction with SWNOM as the idea procedure for application to unknown water samples. Unquenched BSA fluorescence can be calculated by inputting as measured BSA fluorescence at excitation/emission (Ex/Em) pair of 280/344 nm and SWNOM fluorescence at Ex/Em

pair of 350/450 nm into the proposed equation. The unquenched BSA fluorescence from the proposed equation fitted well with the unquenched BSA fluorescence from the experiment with correlation coefficient of determination ( $R^2$ ) of 0.98 and mean absolute error of 0.33 raman unit (RU).

Chapter 6 is the generation of the models for prediction of three sub-species of THMs including chloroform, bromodichloromethane and dibromochloromethane (Bromofrom was under detection limit) of synthesis water samples by using EEM with correction of fluorescence quenching and bromide ion (Br<sup>-</sup>) concentration. The use of proposed models for the prediction of each of three sub-species of THMs increased the prediction accuracy by reducing the error comparing with other existing models using other type of water quality parameters as THM species precursor (e.g., DOC).

Chapter 7 is the overall conclusion of this thesis and the recommendation for future study. As an overall conclusion, the correction of fluorescence quenching plays an important role on the improvement of the prediction accuracy of THMs. Thus, the measured intensity of fluorescence in the protein-like regions are recommended to correct the quenching effect before using as the predictor of THMs in the predictive models. However, the proposed models in this study were derived from the specific compound combination and reaction conditions. Thus, the future studies are recommended for the generalization of the models to be more applicable with the real water condition.

備考 : 論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。

Note : Thesis Summary should be submitted in either a copy of 2000 Japanese Characters and 300 Words (English) or 1copy of 800 Words (English).

注意:論文要旨は、東工大リサーチリポジトリ(T2R2)にてインターネット公表されますので、公表可能な範囲の内容で作成してください。 Attention: Thesis Summary will be published on Tokyo Tech Research Repository Website (T2R2).