

UNIVERSITI TEKNOLOGI MARA

**APPLICATION OF CHEMOMETRICS IN
IDENTIFYING SOURCES OF ORGANIC
CONTAMINANTS IN LANGAT RIVER
BASIN**

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Thesis submitted in fulfilment
of the requirements for the degree of
Master of Science

Faculty of Applied Sciences


March 2015

AUTHOR'S DECLARATION

I declare that the work in this thesis was carried out in accordance with the regulations of Universiti Teknologi MARA. It is original and is the result on my own work, unless otherwise indicated or acknowledged as referenced work. This thesis has not been submitted to any other academic institution or non-academic institution for any other degree or qualification.

I, hereby, acknowledge that I have been supplied with the Academic Rules and Regulations for Post Graduate, Universiti Teknologi MARA, regulating the conduct of my study and research.

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ABSTRACT

With the rapid economic development in Malaysia, environmental pollution has become a major concern, particularly pollution by organic contaminants. Monitoring their temporal and spatial distribution resulted in a large and complicated datasets. It is therefore necessary to apply chemometric techniques to the dataset in order to extract meaningful information and identify the possible sources of these organic contaminants. In this study, the distribution of 13 organic contaminants (polycyclic aromatic hydrocarbons (PAHs), sterols, pesticides (chlorpyrifos), and phenol) in nine monitoring sites along Langat River Basin were monitored from February 2012 to January 2013 on a monthly basis. The analysis of these organic contaminants from surface water was extracted using tandem solid phase extraction (SPE) and analyzed using various chromatographic techniques. The datasets were subjected to chemometric techniques namely hierarchical agglomerative cluster analysis (HACA), discriminant analysis (DA), principal component analysis (PCA) and the factor analysis (FA), to evaluate of possible contamination sources and compared to the inventory of local activities provided by Department of Environmental (DOE), Malaysia. Evaluation on the temporal distribution of these organic contaminants showed that significant variation of PAHs, sterols and phenol during wet weather season (November to April) could be due to dilution factor whereby greater amount of water discharged into the river and intense rainfall could erode the topsoil and carry the accumulated contaminants by surface runoff. By applying HACA, the selected sampling sites were grouped into three clusters which can be correlated to the level of contamination (low, moderate and high contamination sites). Using DA, the contaminants in Langat River could be divided into three sources: domestic sewage/urban discharges, industrial activities and socio-economic activities based on the local activities identified by the Department of Environment (DOE), Malaysia. Forward and backward stepwise DA was able to discriminate two and five organic contaminants variables, respectively, from the original 13 selected variables. The five significant variables identified using backward stepwise DA were fluorene, pyrene, stigmastanol, stigmasterol and phenol. PCA and FA (varimax functionality) were used to identify the possible sources of each organic contaminant based on the inventory of local activities. Five principal components were obtained with 66.5% of the total variation. Result from FA indicated that PAHs (pyrene, fluorene, acenaphthene, benzo[a]anthracene) originated from industrial activity and socio-economic activities; while sterols (coprostanol, stigmastanol and stigmasterol) were associated to domestic sewage and local socio-economic activities. The occurrence of chlorpyrifos was correlated to agricultural activities, urban and domestic discharges. This study showed that the application of chemometrics on the distribution of selected organic contaminants was able to trace the sources of contamination in surface water. In addition, selected pharmaceuticals known as emerging contaminants were determined in samples of surface water of Langat River Basin. Thus, a HPLC separation of six pharmaceuticals (caffeine, acetaminophen, carbamazepine, naproxen, diclofenac and ibuprofen) was developed using two columns (AcclaimTM TrinityTM P1 and AcclaimTM 120 C₁₈). Detectable concentrations of caffeine, acetaminophen, naproxen and diclofenac suggest that these organic contaminants could be a potential chemical marker for domestic sewage. This study showed that the combination of the distribution of organic contaminants and chemometric techniques is a promising approach in identifying the sources of contamination and this information would be helpful for the local authorities to take action in managing environmental pollution.

ACKNOWLEDGEMENTS

Alhamdulillah, by the name of Allah the Almighty, the Most Compassionate, the Most Gracious and the Most Merciful, all praise to Allah for giving me the physical and mental ability upon completion of this thesis.

I would like to express my deepest gratitude to my supervisor, Professor Dr. Norashikin Saim, for her excellent guidance, caring, patience, and providing me with an excellent atmosphere for doing research. My appreciation also goes to my co-supervisor, Dr. Rozita Osman for her guidance, encouragement and valuable advice throughout this study. I would like to express my gratitude to the Dean, School of Postgraduate Studies and Head Programme Department, for their support and help towards my postgraduate affairs. I would like to thank all the officers from Alam Sekitar Malaysia (ASMA) and Faradiah Md. Dali from Universiti Putra Malaysia their assistance in sampling of water samples of Langat River. Sincere thanks to all my friends, Licaberth Ismail, Nazarudin Ibrahim, Nurliayana Ibrahim, Solehatun Mhd. Bani, Siti Norbayu Subari, Syafinaz Abd Aziz, Siti Aisyah Aliasak and Habsah Zahari for their moral support and guidance during my study. I warmly thank Mrs. Noor Haida Kamalul Khudzri, Mrs Roslizawati Ishak and Mr. Ahmad Khambali Khalil and Mr. Dzhahir Dzaidanee Nasaruddin for their assistance during my research.

Finally, special thanks to my beloved family especially my father (Mr. Mohamed Zubir Adon Shah), mother (Rokiah Azahab) and siblings who always support me and for their patience until I completed my study successfully.

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