Behaviour and Health Risk Assessment of Endocrine Disrupting Chemicals from Wastewater

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Abstract

Water supply has become a social and economic issue in many countries as a result of global climate change, fast population growth, industrial and urban development. To address this issue, water recycling has been considered as a feasible technology to supplement the existing water supply. However, a major challenge with water recycling is the removal of harmful contaminants to meet drinking water guidelines and industrial requirements. Although various technologies can remove most contaminants efficiently, recent studies have shown that many endocrine disrupting chemicals (EDCs) can cause adverse health effects on wildlife species and humans at extremely low level.

EDCs from wastewater treatment effluent are the major point source entering the aquatic environment. Consequently, various adverse health effects have been observed in wildlife species, such as population changes, reproductive abnormalities, imbalanced sex ratios and behaviour changes. Many adverse human health effects such as prostate cancer, breast cancer and birth defects have also been implicated with the exposure to EDCs. Thus, it is important to study these environmental contaminants. The main aim of this work was to develop an understanding of the behaviour and health risks of EDCs from wastewater. This work focused on four estrogens, estrone (E1), 17β-estradiol (E2), estriol (E3), and 17α-ethinylestradiol (EE2) and three phenolic compounds, nonylphenol (NP), octylphenol (OP) and bisphenol A (BPA).

The behaviour of a chemical in the environment is largely dependent on its physicochemical properties such as aqueous solubility (S) and octanol-water partition coefficient (K_{ow}). Physicochemical properties, however, are related to chemical
structures. A quantitative structure-property relationship (QSPR) evaluation was conducted by using measured physicochemical properties and calculated molecular descriptors. With single and multiple linear regression methods, good linear relationships were found between the measured log $K_{ow}$ values and three molecular descriptors: log FOSA (hydrophobic component of the total solvent accessible surface area), log FISA (hydrophilic component of the total solvent accessible surface area) and log PSA (Van de Waals surface area of polar nitrogen and oxygen atoms). Similar but weaker correlations were found between the measured log $S$ values and each of the three molecular descriptors. The relationships can be used to obtain property values for various steroidal EDCs which may have potential environmental effects.

The behaviour of EDCs is also affected by some environmental parameters such as temperature, pH and equivalent biomass concentration (EBC). Several authors have noticed the effects of biomass concentration on degradation rate, but quantitative relationships have not been developed. So, this work conducted relationship studies between the measured degradation rate constants and EBC values. Simple linear regression indicated that the degradation rate constant generally increases with higher EBC values. Results showed that EE2 was most resistant to biodegradation, whilst E1 and E2 were relatively easily degraded at similar rates. The relationships obtained are useful for the prediction of the fate of steroidal EDCs in environmental media.

Often, the environmental fate of EDCs cannot be easily measured and mathematical simulation methods have to be used. A fugacity-based model was used to quantify the fate of E1, E2 and EE2 in a reservoir receiving recycled water in Queensland, Australia.
Under typical conditions, the simulated concentration in water after advanced water treatment were below $10^{-4}$ ng/L, implying negligible health risk when compared with no-observed-adverse-effects-concentration (NOAEC) for fish and Australia Public Health Standards (PHS) for humans. In addition, the simulated concentrations in water decreased when water temperature, reservoir water storage volume, EBC and reservoir water releasing rate increased. However the opposite trend was found with wastewater recycling rate and EDC concentration in the final recycled water.

To conduct health risk assessment for fish and humans, probabilistic techniques were used. A new risk characterisation method, the overall risk probability (ORP) was developed based on the cumulative probability distribution (CPD) of exposure and effect data. The ORP method obtained the same ranking of risk level for fish as the commonly used hazard quotient (HQ$_{95/5}$) method: EE2 (HQ$_{95/5}$, 250; ORP, 26.6%) > E1 (HQ$_{95/5}$, 63; ORP, 22.0%) > E2 (HQ$_{95/5}$, 16; ORP, 8.1%) > E3 (HQ$_{95/5}$, 1.2; ORP, 3.8%) > NP (HQ$_{95/5}$, 0.46; ORP, 0.6%) > BPA (HQ$_{95/5}$, 0.084; ORP, 0.4%) > OP (HQ$_{95/5}$, 0.057; ORP, 0.2%). All calculated HQ$_{95/5}$ and ORP values for estrogens were above their respective reference value of 1 in the HQ$_{95/5}$ method and 2.5% in the ORP method, implicating the contamination in surface water by estrogens is a global issue of concern. Due to the lack of human effect data, the ORP method was not used in human risk characterisation. Instead, the risk was quantified using acceptable daily intake (ADI) values developed by international and Australian agencies, which gave the ranked HQ$_{95/ADI}$ values in the order of E1 (3.16) > E2 (1.09) > BPA (0.200) > EE2 (0.0398) ≈ E3 (0.0398) > NP (0.0200) > OP (0.00252) for international ADI values and E1 (36.8) > EE2 (0.926) > E2 (0.632) > E3 (0.284) > BPA (0.200) > OP (0.00839) > NP (0.00667)
for Australian ADI values. Apparently, with both sets of ADI values, the HQ<sub>95/ADI</sub> values obtained for E1 were above the reference value of 1, showing significant level of risk to human health. Compared with the single-point HQ<sub>95/5</sub> method, the ORP method demonstrated the capability to reflect the information in the shape of cumulative distribution curves. Therefore, it is regarded as an improvement in risk characterisation.
Statement of originality

“This work has not been previously submitted for a degree or diploma in any university. To the best of my knowledge and belief, this thesis contains no material previously published or written by another person except where due reference is made in the thesis itself”.

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Signature

August 2010
Acknowledgments

I would like to express most sincere gratitude to my principal supervisors Dr. Jimmy Yu and Professor Des Connell. Their kind guidance and suggestions to my research project were invaluable. They have given me enormous amount of encouragement and assistance. They have taught me how to prioritize on tasks, how to organize ideas, how to manage time and cost. Most importantly, they taught me how to think critically. Their teachings will continue to benefit my future work.

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<th>Description</th>
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<tbody>
<tr>
<td>ADI</td>
<td>Acceptable Daily Intake</td>
</tr>
<tr>
<td>APEO</td>
<td>Alkylphenol Ethoxylates</td>
</tr>
<tr>
<td>AWTP</td>
<td>Advanced Wastewater Treatment Plant</td>
</tr>
<tr>
<td>BCF</td>
<td>Bioconcentration Factor</td>
</tr>
<tr>
<td>BOD</td>
<td>Biological Oxygen Demand</td>
</tr>
<tr>
<td>BPA</td>
<td>Bisphenol A</td>
</tr>
<tr>
<td>cfu</td>
<td>Colony-forming Unit</td>
</tr>
<tr>
<td>CP</td>
<td>Cumulative Probability</td>
</tr>
<tr>
<td>CPD</td>
<td>Cumulative Probability Distribution</td>
</tr>
<tr>
<td>DDT</td>
<td>Dichlorodiphenyltrichloroethane</td>
</tr>
<tr>
<td>DES</td>
<td>Diethylstilbestrol</td>
</tr>
<tr>
<td>E1</td>
<td>Estrone</td>
</tr>
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<td>E2</td>
<td>17β-estradiol</td>
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<td>Estriol</td>
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<tr>
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<td>17α-ethinylestradiol</td>
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<td>EBC</td>
<td>Equivalent Biomass Concentration</td>
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<tr>
<td>BC</td>
<td>Biomass Concentration</td>
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<tr>
<td>EDCs</td>
<td>Endocrine Disrupting Chemicals</td>
</tr>
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<td>EE2</td>
<td>17α-ethinylestradiol</td>
</tr>
<tr>
<td>EEF</td>
<td>Estradiol Equivalent Factor</td>
</tr>
<tr>
<td>EEQ</td>
<td>Estradiol Equivalent Quantity</td>
</tr>
<tr>
<td>FISA</td>
<td>Hydrophilic Component of the Total Solvent Accessible Surface Area</td>
</tr>
<tr>
<td>FOSA</td>
<td>Hydrophobic Component of the Total Solvent Accessible Surface Area</td>
</tr>
<tr>
<td>H</td>
<td>Henry’s Law Constant</td>
</tr>
<tr>
<td>HC</td>
<td>Hazard Concentration</td>
</tr>
<tr>
<td>HDD</td>
<td>Human Daily Dose</td>
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<td>Human Equivalent Dose</td>
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<td>HQ</td>
<td>Hazard Quotient</td>
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<tr>
<td>Abbreviation</td>
<td>Term</td>
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<tr>
<td>--------------</td>
<td>------</td>
</tr>
<tr>
<td>HRT</td>
<td>Hydraulic Retention Time</td>
</tr>
<tr>
<td>k</td>
<td>Degradation Rate Constant</td>
</tr>
<tr>
<td>$K_{oc}$</td>
<td>Octanol-Carbon Partition Coefficient</td>
</tr>
<tr>
<td>$K_{ow}$</td>
<td>Octanol-Water Partition Coefficient</td>
</tr>
<tr>
<td>LOAEC</td>
<td>Lowest-Observed-Adverse-Effects-Concentration</td>
</tr>
<tr>
<td>MF</td>
<td>Microfiltration</td>
</tr>
<tr>
<td>MLSS</td>
<td>Mixed Liquor Suspended Solids</td>
</tr>
<tr>
<td>MLVSS</td>
<td>Mixed Liquor Volatile Suspended Solids</td>
</tr>
<tr>
<td>MOS</td>
<td>Margin of Safety</td>
</tr>
<tr>
<td>MW</td>
<td>Molecular Weight</td>
</tr>
<tr>
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<td>Nitrifying Activated Sludge</td>
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<td>Overall Risk Probability</td>
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Publications arising from this work


