International Biodeterioration & Biodegradation xxx (2017) 1–5

Contents lists available at ScienceDirect

International Biodeterioration & Biodegradation

journal homepage: www.elsevier.com/locate/ibiod

Toxicity evaluation of five polyaromatic hydrocarbons to *Escherichia coli* using microcalorimetry and QASRs

Xiaoying Wu [a, b], Jun Yao [a, c, d, *], Fei Wang [a], Jiaheng Ma [a], Jingjing Sun [a], Ruiping Liu [a]

[a] School of Energy and Environmental Engineering and National "International Cooperation Based on Environment and Energy", Beijing Key Laboratory of Resource-oriented Treatment of Industrial Pollutants, University of Science and Technology Beijing, 100083 Beijing, PR China
[b] CIECC Overseas Consulting Co., Ltd., 100048, Beijing, PR China
[c] State Key Laboratory of Biogeology and Environmental Geology, Sino-Hungarian Joint Laboratory of Environmental Science and Health, University of Geosciences, Wuhan 430074, PR China
[d] School of Water Resource and Environmental Engineering, Sino-Hungarian Joint Laboratory of Environmental Science and Health, China University of Geosciences (Beijing), 29 Xueyuan Road, Haidian District, 100083 Beijing, PR China

ARTICLE INFO

Article history:
Received 28 April 2016
Received in revised form
15 January 2017
Accepted 16 January 2017
Available online xxx

Keywords:
Polyaromatic hydrocarbons
Escherichia coli
Microcalorimetry
Toxicity
Quantitative Structure–Activity Relationships (QASRs)

ABSTRACT

The toxicity of five polyaromatic hydrocarbons (PAHs) to metabolism of *Escherichia coli* (*E. coli*) was evaluated with key parameters, including growth constant (*k*) and inhibitory ratio (*I*) from microcalorimetry analysis. The results showed that the toxicity followed pyrene > 9-phenanthrol > phenanthrene > 3-phenanthrenecarboxylic acid > naphthalene for the chemicals tested. Basing on physical and chemical parameters of these five PAHs, the quantitative structure–activity relationships (QASRs) equation was established by multiple linear regression analysis, indicating that narcosis, a non-specific and non-reactive toxic action, plays the predominant role in toxicity of these five PAHs to bacterial cells. This study illustrates that the toxicity of PAHs are determined by the number of the aromatic ring and the substituent groups, higher toxicity associated with the higher number of the aromatic rings.

1. Introduction

Polycyclic aromatic hydrocarbons (PAHs), ubiquitous in natural environment, are major environmental pollutants because they are toxic, carcinogenic, teratogenic, and mutagenic (Edwards, 1983; Obuekwe and Semple, 2013 Gatheru et al., 2015). PAHs are produced diversely when hydrocarbons are not completely burned or mineralized (Geldenhuys et al., 2015; Wang and Simoneit, 1991).

The toxicity of PAHs decreases after degradation in most of the cases, but there are exceptions to this. Degradation of different PAHs leads to variety of degradation intermediates: the degradation intermediates of phenanthrene and pyrene are 3-phenanthrenecarboxylic and 9-phenanthrol, respectively (Xiao et al., 2012). Degradation products of PAHs may result in more toxic intermediates, increasing the health risks to organisms, including humans, which deserves further study (Hamdi et al., 2012; Sun et al., 2015). The toxicity of PAHs and their degradation intermediates may vary due to the differences in molecule structures. Over the past decades, the toxic impact of pyrene, phenanthrene, naphthalene to microorganisms has been extensively studied (Liao et al., 2008; Wu et al., 2013). However, few investigations have shown the toxicity of degradation intermediates of phenanthrene to microorganisms through the observation of microbial metabolic activities directly. *E. coli* is a model laboratory microorganism that has been previously used for evaluating the toxicity of organic compounds (Sandy et al., 2010).

Microbial metabolic activity is an effective microbial index to assess the toxicity of chemicals (Braissant et al. 2013, 2015). Meanwhile, QSARs was also reported according to the microbial metabolic activity parameters and physiochemical properties of a series of chemicals (Li et al., 2010a). The information of such study may provide further insights to the basic understanding of microbial ecotoxicology to allow the development of this field to better understand and protect the physical environment from pollutants (Cheung and Gu, 2007; Gu, 2016; Gu and Wang, 2012, 2013; 2014).

The objectives of this study were analysis of the toxicity of five

* Corresponding author. University of Science and Technology Beijing, 30 Xueyuan Road, Beijing 100083, PR China.
E-mail addresses: yaojun@ustb.edu.cn, yaojun@cug.edu.cn (J. Yao).

http://dx.doi.org/10.1016/j.ibiod.2017.01.030
0964-8305/

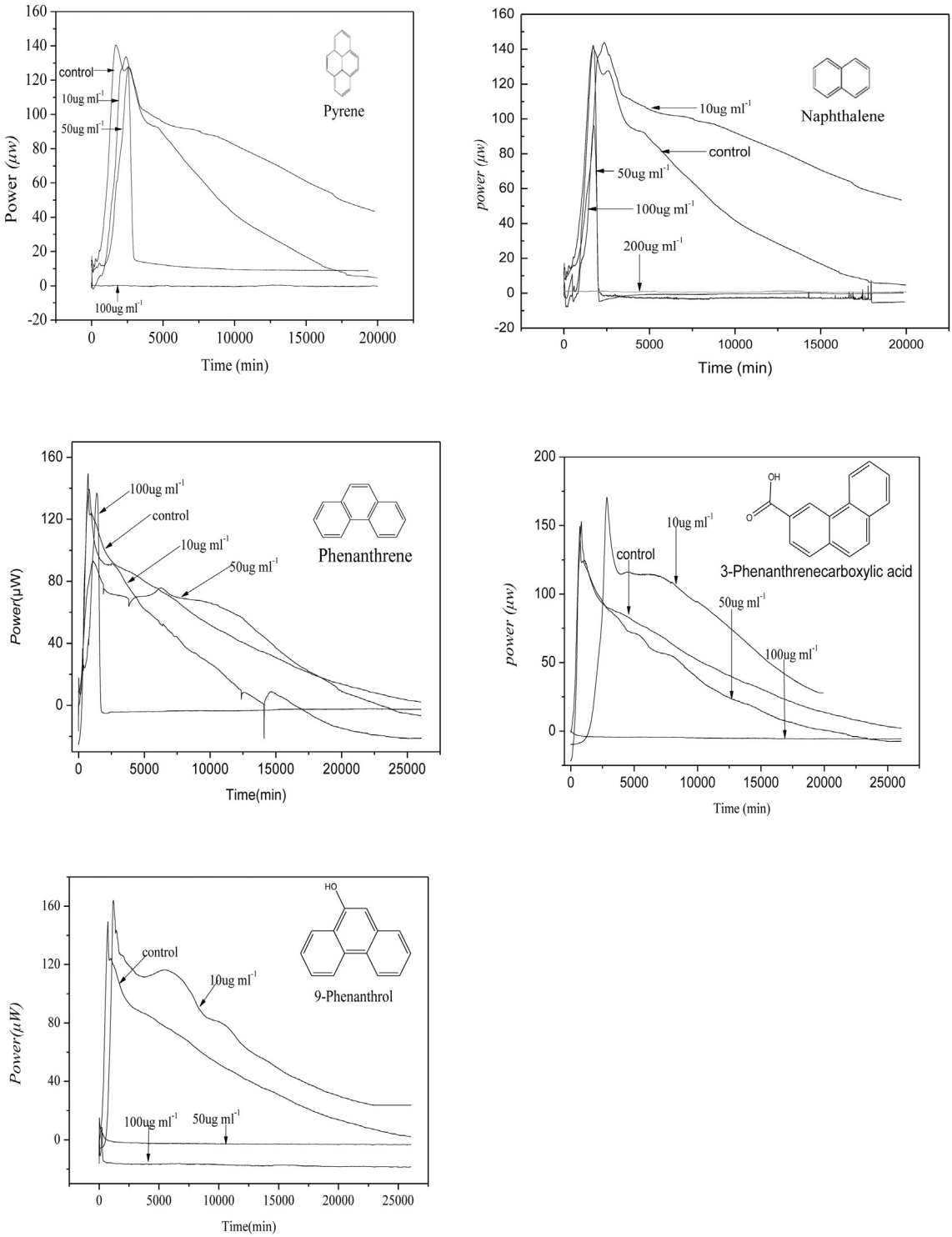

Fig. 1. Power–time curves of *E. coli* at different concentration of pyrene, naphthalene, phenanthrene, 3-phenanthrenecarboxylic, 9-phenanthrol.

PAHs to *E. coli* by microcalorimetry, establishment of QSARs based on the biological process observed, and explanation of the toxic effects of PAHs and their degradation intermediates.

2. Materials and method

2.1. Materials

The *E. coli* strain for this study was obtained from the Institute of Microbiology, Chinese Academy of Science. The chemicals obtained from the Sinopharm Chemical Reagent Co., Ltd. included pyrene, naphthalene, phenanthrene, 9-phenanthrol, 3-phenanthrenecarboxylic acid with 99% purity. The stock solution was prepared to dissolve each of the five chemicals in methanol (5000 mg l^{-1}), then the bacterial culture medium was diluted to designated concentrations (0, 10, 50, 100, and 200 mg l^{-1}). The testing procedures were described previously (Sandy et al., 2010; Folwell and McGenity, 2016).

Please cite this article in press as: Wu, X., et al., Toxicity evaluation of five polyaromatic hydrocarbons to *Escherichia coli* using microcalorimetry and QASRs, International Biodeterioration & Biodegradation (2017), http://dx.doi.org/10.1016/j.ibiod.2017.01.030