Review

A synthesis of parameters related to the binding of neutral organic compounds to charcoal

Sarah E. Hale [a,*], Hans Peter H. Arp [a], Darya Kupryianchyk [a], Gerard Cornelissen [a,b,c]

[a] Department of Environmental Engineering, Norwegian Geotechnical Institute (NGI), P.O. Box 3930, Ullevål Stadion, N-0806 Oslo, Norway
[b] Department of Plant and Environmental Sciences (NMBU), Norwegian University of Life Sciences, 5003 Ås, Norway
[c] Department of Applied Environmental Sciences (ITM), Stockholm University, 10691 Stockholm, Sweden

HIGHLIGHTS

- Charcoal-water partitioning coefficients (K_D values) were compiled from the literature.
- K_D values were correlated with charcoal and organic compound properties.
- Production temperature and surface area were most strongly correlated with K_D.

GRAPHICAL ABSTRACT
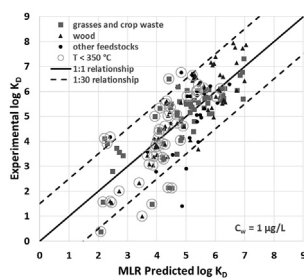
ARTICLE INFO

ABSTRACT

The sorption strength of neutral organic compounds to charcoal, also called biochar was reviewed and related to charcoal and compound properties. From 29 studies, 507 individual Freundlich sorption coefficients were compiled that covered the sorption strength of 107 organic contaminants. These sorption coefficients were converted into charcoal–water distribution coefficients (K_D) at aqueous concentrations of 1 ng/L, 1 µg/L and 1 mg/L. Reported log K_D values at 1 µg/L varied from 0.38 to 8.25 across all data. Variation was also observed within the compound classes; pesticides, herbicides and insecticides, PAHs, phthalates, halogenated organics, small organics, alcohols and PCBs. Five commonly reported variables; charcoal production temperature T, surface area SA, H/C and O/C ratios and organic compound octanol–water partitioning coefficient, were correlated with K_D values using single and multiple-parameter linear regressions. The sorption strength of organic compounds to charcoals increased with increasing charcoal production temperature T, charcoal SA and organic pollutant octanol–water partitioning coefficient and decreased with increasing charcoal O/C ratio and charcoal H/C ratio. T was found to be correlated with SA ($r^2 = 0.66$) and O/C ($r^2 = 0.50$), particularly for charcoals produced from wood feedstocks ($r^2 = 0.73$ and 0.80, respectively). The resulting regression: log $K_D = (0.18 \pm 0.06)$ log $K_{ow} + (5.74 \pm 1.40)$ log T + (0.85 ± 0.15) log SA + (1.60 ± 0.29) log OC + (-0.89 ± 0.20) log HC + (-13.20 ± 3.69), $r^2 = 0.60$, root mean squared error = 0.95, n = 151 was obtained for all variables. This information can be used as an initial screening to identify charcoals for contaminated soil and sediment remediation.

© 2015 Elsevier Ltd. All rights reserved.

* Corresponding author.
  E-mail address: sarah.hale@ngi.no (S.E. Hale).

Contents

1. Introduction

Charcoal is the solid product formed during the incomplete combustion (pyrolysis) of biomass and is also referred to as biochar. Interest in biochar has increased dramatically in recent years owing in principle to the many touted environmental benefits of its use as a soil amendment (Lehmann, 2007). Charcoal can contribute to the mitigation of climate change (by sequestering carbon and suppressing nitrous oxide emissions) (Rondon et al., 2007; Yanai et al., 2007) and specifically when added to acidic soils with low pH and often low cation exchange capacity (CEC), it can improve the agricultural properties of these soil, as charcoal is able to increase pH and cation exchange capacity (CEC) (Liang et al., 2006). In addition, charcaol is able to improve plant available water (Glaser et al., 2002), improve mycorrhizal interactions (Warnock et al., 2007), and provide nutrients that are essential to plant growth (Yamato et al., 2006) to soils with variable physical and biological properties. Charcoal production can be an effective part of agricultural waste management as the process provides a utility for agricultural waste that would otherwise be disposed of and can also generate energy.

In addition to these benefits, many charcoals can strongly sorb organic pollutants (Chen and Chen, 2009; Sun et al., 2012a,b) as well as some metals (Zheng et al., 2012; Khan et al., 2013) and thus for certain types of pollutants and soils or sediments, charcoal amendments could be used for contaminant remediation (Ahmad et al., 2014). Similar to activated carbon (a man-made material and produced from biomass or anthracite coal and exposed to an activation process), charcoal could thus be added to polluted soils and sediments as a way to sequester pollutants, thereby hindering them from leaching or being taken up by organisms (Zimmerman et al., 2005; Ghosh et al., 2011). Charcoal is a form of black carbon (as is activated carbon), composed of rigid and planar stacks of highly disordered polyaromatic hydrocarbon sheets (graphene) with relatively few polar functionalities (ketone, ether, hydroxyl, quinoid, carboxyl and other functional groups) on its surface compared to other forms of soil organic matter (e.g. humus) (Cornelissen et al., 2005). Black carbon materials (including charcoal) have high carbon contents, large microporous networks and high surface areas (Allen-King et al., 2002; Zhu and Pignatello, 2005). These properties not only render charcoal resistant

to chemical and microbial degradation (Spokas, 2010), where half-lives of between 8 and 4000 years have been reported for charcoals (Gurwick et al., 2013), but are also responsible for the high sorption strength of organic compounds to charcoal.

Sorption to soils and sediments is one of the most important environmental processes related to organic pollutants as it controls their environmental mobility and bioavailability and thus their risk. Sorption to charcoal is expected to be similar to other condensed organic matters such as soot (Jonker and Koelmans, 2002), coal (Cornelissen and Gustafsson, 2005; Yang et al., 2008), kerogen (Cornelissen and Gustafsson, 2005) and lampblack (Hong and Luthy, 2007) based on their similar properties. The sorption of organic pollutants to carbonaceous geosorbents occurs via physisorption (i.e. reversible sorption that does not involve the formation of covalent bonds) on the exterior surface and in meso-, macro- and micropores (Jonker and Koelmans, 2002; Koelmans et al., 2006) and also via pore filling (Kleineidam et al., 2002). During these physisorption processes, intermolecular forces occur between charcoal functional groups and organic pollutants, such as ionic interactions, electron-donor-acceptor (EDA) interactions (e.g. Lewis acid-base (H-bonding) and π–π electron donor-acceptor (EDA) interactions) and van der Waal interactions (i.e. between dipoles, induced dipoles and instantly induced dipoles (i.e. London dispersion)) (Israelachvili, 1992). Previous studies have indicated pore filling, H-bonding interactions and a specific type of EDA interaction known as the π–π EDA interaction are the prominent mechanisms of sorption of organic compounds (Zhu and Pignatello, 2005). Although physisorption processes dominate, chemisorption process may take place and sorb organic pollutants (in their charged state) to carbonaceous geosrbents. Chemisorption involves surface reactions where organic compounds participate in bond-making and bond-breaking processes (Schwarzenbach et al., 2003).

Pore filling occurs when organic pollutants enter micropores within the charcoal structure and can be a descriptive factor in the sorption strength of such materials (Kleineidam et al., 2002). The extent of pore filling is highly dependent on the overlap in size of the organic pollutant and the pore itself. The π–π EDA interaction has been the subject of scrutiny (Grimme, 2008) and involves interactions between a π electron rich donor and a π electron poor acceptor which lead to a π–π EDA stacking interaction (Zhu and Pignatello, 2005). In a charcoal-organic pollutant