Molecular properties affecting the adsorption coefficient of phenylurea herbicides

Alodie Blondel · Julie Langeron · Stéphanie Sayen · Eric Hénon · Michel Couderchot · Emmanuel Guillon

Received: 17 February 2013 / Accepted: 15 March 2013 / Published online: 16 April 2013 © Springer-Verlag Berlin Heidelberg 2013

Abstract The adsorption of 12 pesticides of the phenylurea family was studied by batch experiments in order to determine the adsorption coefficient, \( K_\text{d} \). The study was conducted in two soils chosen for their differences in organic matter and calcite contents. \( K_\text{d} \) pesticide adsorption coefficients were higher for soil S1 than for soil S2 due to the presence of a higher organic matter content and a lower calcite content in soil S1. To identify pesticide properties governing retention, 18 molecular descriptors were considered. Class-specific quantitative structure-property relationship (QSPR) soil sorption models using one, two, and three descriptors were developed from our experimental data using linear regressions. One of the aims of this work was to check whether QSPR models that did not include literature values of \( K_\text{ow} \) were able to predict \( K_\text{d} \) coefficients in satisfactory agreement with our experimental data. The influence of the level of theory in determining \( K_\text{ow} \) and polarisability predictors on the predictive performance of the model was also examined by comparing quantum chemistry and empirical (QikProp) approaches. The one-descriptor model using “quantum” polarisability \( \alpha \) was found to perform almost as well as or better than the other models.

Keywords Soil · Adsorption · Hydrophobicity · \( K_\text{ow} \) · Polarisability · Molecular descriptors · DFT · \( K_\text{d} \)

Introduction

Because of their wide use, pesticides are present in all environmental compartments (Turgut et al. 2010; Messing et al. 2011) and especially in ground and surface waters (Palma et al. 2004; Huber et al. 2000; Morvan et al. 2006). In France, 78,600 t of pesticides were used in 2008 (Catignon and Etienne 2010), and herbicides are among the most utilized molecules, more particularly the phenylurea compounds (Blanchoud et al. 2007). Two phenylureas, isoproturon and diuron, were detected at a level of 248 % of the samples in the Marne River, France; they represent with atrazine and mecoprop 40 % of the total contamination of this river (Blanchoud et al. 2007). Moreover, phenylureas may cause adverse effects on aquatic organisms such as algae (Arrhenius et al. 2004), bivalve species (Damasio et al. 2010) and fish (Tierney et al. 2011), but they also can cause damage on small mammals (Federico et al. 2011) and are suspected to be endocrine disruptors (Orton et al. 2009). Because of their toxicity and their ubiquity in the water resource, phenylurea behaviour in soils is of great interest and has been the object of several studies (Fava et al. 2006; Salvestri et al. 2008). Contamination of water is often the result of transfer through and in the soils to the ground and surface waters.

Dissipation of a pesticide in soils is the result of phenomena such as volatilization (Guzzella et al. 2006), degradation (Hussein et al. 2011) and leaching (Irace-Guigard and Aaron 2003), which in turn is mainly governed by pesticide adsorption in soils (Calvet 1989). To evaluate the adsorption of a