

## Uptake and acropetal translocation of polycyclic aromatic hydrocarbons by wheat (*Triticum aestivum* L.) grown in field-contaminated soil

Tao, Y. Q., Zhang, S. Z., Zhu, Y. G., & Christie, P. (2009). Uptake and acropetal translocation of polycyclic aromatic hydrocarbons by wheat (*Triticum aestivum* L.) grown in field-contaminated soil. *Environmental Science and Technology*, 43(10), 3556-3560. DOI: 10.1021/es803368y

**Published in:**  
Environmental Science and Technology

**Queen's University Belfast - Research Portal:**  
[Link to publication record in Queen's University Belfast Research Portal](#)

### General rights

Copyright for the publications made accessible via the Queen's University Belfast Research Portal is retained by the author(s) and / or other copyright owners and it is a condition of accessing these publications that users recognise and abide by the legal requirements associated with these rights.

### Take down policy

The Research Portal is Queen's institutional repository that provides access to Queen's research output. Every effort has been made to ensure that content in the Research Portal does not infringe any person's rights, or applicable UK laws. If you discover content in the Research Portal that you believe breaches copyright or violates any law, please contact [openaccess@qub.ac.uk](mailto:openaccess@qub.ac.uk).

# Uptake and Acropetal Translocation of Polycyclic Aromatic Hydrocarbons by Wheat (*Triticum aestivum* L.) Grown in Field-Contaminated Soil

YUQIANG TAO,<sup>†</sup> SHUZHEN ZHANG,<sup>\*†</sup>  
YONG-GUAN ZHU,<sup>†</sup> AND  
PETER CHRISTIE<sup>‡</sup>

State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China, and Agri-Environment Branch, Agriculture Food and Environmental Science Division, Agri-Food and Biosciences Institute, Queen's University of Belfast, Newforge Lane, Belfast BT9 5PX, U.K.

Received November 27, 2008. Revised manuscript received March 5, 2009. Accepted March 25, 2009.

Uptake and acropetal translocation of 14 priority polycyclic aromatic hydrocarbons (PAHs) by wheat (*Triticum aestivum* L.) grown in 15 field-contaminated soils were investigated in a growth chamber. PAH concentrations in roots correlated positively with the corresponding concentrations in soils and negatively with the contents of soil organic carbon ( $p < 0.01$ ). No clear linear relationship was found between log RCF (root concentration factor,  $\mu\text{g g}^{-1}\text{root}/\mu\text{g g}^{-1}\text{soil}$  on dry weight basis) and log  $K_{ow}$  of these PAHs. Four-ring PAHs had the highest tendency to be taken up by roots. PAH concentrations in shoots correlated well with their concentrations in soils and roots. Furthermore, distribution profiles of PAHs in shoots were fairly similar to those in soils. Acropetal translocation of 10 PAHs (with log  $K_{ow}$  varying from 3.45 to 5.78) was also implicated by  $R_t$  (ratio of PAH from root-to-shoot translocation to the total accumulation in shoots) ranging from 53.6 to 72.6%. A negative linear relationship was found between log  $R_t$  and log  $K_{ow}$  of these PAHs ( $p < 0.01$ ), and acropetal translocation of PAHs depended on their chemical properties.

## Introduction

Uptake of hydrophobic organic compounds (HOCs) such as polycyclic aromatic hydrocarbons (PAHs) by plants may occur through soil-to-plant and air-to-plant pathways, including root uptake and atmospheric deposition from gaseous or particulate forms (1, 2). HOCs with high hydrophobicity in soils are strongly associated with soil and particularly with soil organic matter, and only a very limited fraction would be expected to be available for plant uptake (1, 3). After uptake by roots, these compounds partition strongly onto the root epidermis and will be translocated to shoots with difficulty (4–6). As a consequence, HOCs in above-ground plant tissues are considered to be mainly derived from the atmosphere (4).

However, recent studies have indicated that HOCs (including PAHs) are transported to the shoots of some plant species through the soil-to-plant pathway. Hülster et al. (7) found that zucchini (*Cucurbita pepo* L. convar. *gironmontina*) and pumpkins (*C. pepo* L. cv. Gelber Zentner) could take up and translocate large amounts of PCDD/Fs from contaminated soils and root uptake was the main uptake pathway for these plant species. Zucchini also took up DDE (8) through a soil-to-plant exposure pathway. Chlordane detected in the shoots of spinach, lettuce, dandelion, and zucchini was reported to be taken up by roots from soils (9, 10). By investigating soil-to-root transfer and translocation of PAHs by vegetables grown on industrially contaminated soils, Fismes et al. (1) concluded that root uptake was the main pathway for high molecular weight PAHs while lower molecular weight PAHs were likely taken up both from the atmosphere through the leaves and by roots. However, there are conflicting reports in the literature concerning the extent of uptake and translocation of HOCs from roots to shoots (1, 11, 12). Whether compounds with intermediate and high hydrophobicity such as a series of PAHs can acropetally translocate in plants has not yet been verified. Furthermore, it needs to be clarified how much HOC in roots can be translocated from roots to aerial tissues. Particular attention should be paid to plants grown in field-contaminated soil. Two-photon excitation microscopy coupled with autofluorescence (TPEM-AF) has provided a powerful technique that enables the visualization and tracking of how organic pollutants are taken up into plants and how they behave once within the living plant tissues (13). Wild and his co-workers have pioneered the use of this technique to track the uptake and movement of PAH inside living plant leaves (14) and roots (15). They observed that for root uptake the PAHs anthracene and phenanthrene initially bound to the epidermis along the zone of elongation, passing through the epidermal cells to reach the cortex within the root hair and branching zones of the root. The PAHs entered the epidermis radially, and once within the cortical cells this movement was dominated by a slow lateral movement toward the shoot (14). For leaf uptake, anthracene was evidenced to move through the epicuticular wax and plant cuticle, reaching the cytoplasm of the epidermal cells (15). However, it is not clear whether the technique is suitable for quantifying the uptake and in particular the translocation of a series of compounds inside plants.

Physicochemical properties of HOCs may affect their uptake by roots and subsequent translocation within the plants. Previous studies (6, 16) have sought to explore the relationship between root concentration factor (RCF) and hydrophobicity. However, a positive linear relationship between log RCF and log  $K_{ow}$  has been established for the uptake of only a few hydrophilic nonionized compounds by several plant species in hydroponic experiments. Information is very limited about the influence of hydrophobicity of a series of compounds with intermediate and high lipophilicity on their uptake and translocation by plants, particularly by plants growing in field-contaminated soils.

Therefore, the aim of the present study was to investigate the uptake and acropetal translocation of 14 priority PAHs by plants from soil. Wheat (*Triticum aestivum* L.) was selected as the model plant because it is a widely cultivated and important monocotyledonous crop species. Fifteen field-contaminated soils were used to explore the influences of physicochemical properties of soils and PAHs on the uptake and acropetal translocation of PAHs by wheat.

\* Corresponding author phone: +86-10-62849683; fax: +86-10-62923563; e-mail: szzhang@rcees.ac.cn.

<sup>†</sup> Chinese Academy of Sciences.

<sup>‡</sup> Queen's University of Belfast.

## Materials and Methods

**Chemicals and Solvents.** The 14 priority PAHs were naphthalene (Nap), acenaphthene (Ace), fluorene (Flu), phenanthrene (Phe), anthracene (Ant), fluoranthene (Fla), pyrene (Pyr), benzo[*a*]anthracene (BaA), chrysene (Chr), benzo[*b*]fluoranthene (BbF), benzo[*k*]fluoranthene (BkF), benzo[*a*]pyrene (BaP), dibenzo[*a,h*]anthracene (DahA), and benzo[*g,h,i*]perylene (BghiP). Acenaphthylene (Acy) was excluded from this study because of its low fluorescence. Indeno[1,2,3-*cd*]pyrene was also excluded because it was below the detection limit in several field-contaminated soils used in the study. The PAHs were grouped according to their ring number. Standard solutions of 16 priority PAHs (200  $\mu\text{g L}^{-1}$ ) with purity >99% were purchased from Acros Organics and used for identification and quantification. All solvents used (i.e., *n*-hexane, dichloromethane, acetonitrile, chloroform, and methanol) were of HPLC grade.

**Soil Preparation.** Samples of the 15 field-contaminated soils were collected from the 5–25-cm depth zone of agricultural fields near Tianjin city in northern China where PAHs occur in many locations as a result of coal, petroleum and biomass combustion, and wastewater irrigation over several years or decades (17). Each soil sample was air-dried, passed through a 2-mm sieve, sterilized by  $\gamma$ -irradiation from a  $^{60}\text{Co}$  source, and stored in brown glass containers at room temperature. Before plant cultivation experiments, concentrations of PAHs in soils were determined, content of total organic carbon (TOC) in the soils was determined by the Walkley–Black method (18), and content of dissolved organic carbon (DOC) was determined with a TOC analyzer (Phoenix 8000). Sampling locations and DOC and TOC contents in the soils are listed in Table S1 in the Supporting Information. Concentrations of PAHs in the soils are presented in Table S2 in the Supporting Information.

**Wheat Cultivation and Characterization.** Wheat seeds (*T. aestivum* L., obtained from the Chinese Academy of Agricultural Sciences, Beijing, China) were first surface sterilized in 3%  $\text{H}_2\text{O}_2$ , soaked in 2.8  $\text{mmol L}^{-1}$   $\text{Ca}(\text{NO}_3)_2$  for 4 h, and then germinated in a cultivation dish by placing them on moist filter paper at 22–27 °C. After germination, uniform seedlings were selected and transferred to plastic pots (3 plants  $\text{pot}^{-1}$ ) uniformly packed with 300 g of field-contaminated soil. The seedlings were grown under plant growth chamber conditions for 14 h at 27 °C (day cycle) and for 10 h at 22 °C (night cycle). Plants were irrigated daily with distilled water to maintain soil moisture at 30% by weight. Three replicates were set up for each soil. In parallel, wheat cultivation in hydroponic solution without PAH addition was conducted to estimate gaseous uptake of PAHs into wheat shoots (16) and glass plates filled with XAD-2 resin were placed in the growth chamber to sample PAHs from the ambient air in the plant growth chamber (1). Various treated pots, controls in hydroponic solution, and XAD-2 resin were randomized in the plant growth chamber side by side and were rerandomized frequently, and the PAH concentrations in the air would have quickly become homogeneous after volatilizing from soils. Plants were harvested after cultivation for 45 days, and the XAD-2 resins were collected at the same time as plant harvest. Roots and shoots were separated after harvest. They were first washed thoroughly with tap water and then with distilled water, wiped with clean filter paper and weighed immediately, and finally freeze-dried for 72 h and weighed again. The dried samples were cut with stainless steel scissors and ground in a mortar to obtain homogeneous samples.

Lipid content of roots and shoots was determined by Soxhlet extraction with 100 mL of mixed solvent of chloroform and methanol (2:1, v/v) for 24 h. The extract was dried in a rotary evaporator, redissolved in 20 mL of *n*-hexane, filtered through No. 5 Whatman filter paper into a preweighed glass

tube to remove precipitates, and dried to a constant weight. The weight of the residue was considered as the lipid (19). The water contents of roots and shoots were  $82.07 \pm 1.34$  and  $80.74 \pm 0.65$  wt %, and the lipid contents of roots and shoots were  $1.14 \pm 0.3$  and  $0.67 \pm 0.1$  wt %, respectively.

**Chemical Analysis.** Samples of soil, roots, shoots, and XAD-2 resin from triplicate pots of the treatments were collected. Each subsample (0.1 g of dry weight) was thoroughly mixed with 1–2 g of anhydrous sodium sulfate, loaded into a Soxhlet thimble, and extracted with 100 mL of *n*-hexane/dichloromethane (1:1 v/v) at 60 °C for 24 h. The extract was reduced to about 5 mL with a rotary evaporator, purged to about 1–2 mL under a gentle nitrogen stream, and then cleaned with a Florisil SPE (1 g/6 mL) and eluted with 6 mL of *n*-hexane/dichloromethane (4:1 v/v). The eluates were evaporated, solvent-exchanged into methanol (1.00 mL), and stored before analysis.

PAHs in samples were analyzed by HPLC-FLD (Agilent 1200 series). Chromatographic separation and resolution were best achieved by using a LiChrospher (Merck) reverse-phase  $\text{C}_{18}$  column (4.6  $\times$  250 mm, 5- $\mu\text{m}$  particle size) specific for PAH analysis with the mobile phase of acetonitrile/water (0.75 mL/min, 0–10 min 60:40, 10–50 min from 60:40 to 100:0, post run 5 min). The  $\text{C}_{18}$  column was kept at 25 °C. The excitation wavelength was 260 nm. The emission wavelength of Nap, Ace, Flu, and Phe was 380 nm, and for the other PAHs it was 420 nm.

Results were obtained from three replicate pots of each treatment for soils, roots, shoots, and XAD-2 resin. Solvent, root, and shoot controls were included. A linearity higher than 0.990 for the concentrations of standard sample varying from 8 to 100  $\mu\text{g L}^{-1}$  was obtained, and detection limits ( $S/N = 3$ ) were as low as 2.1, 2.2, 6.1, 0.25, 1.6, 1.5, 4.1, 0.52, 0.93, 3.03, 0.08, 5.7, 0.08, and 2.3  $\mu\text{g L}^{-1}$  for Nap, Ace, Flu, Phe, Ant, Fla, Pyr, BaA, Chr, BbF, BkF, BaP, DahA, and BghiP, respectively, under the HPLC-FLD conditions used in this study. Extraction recoveries were determined by spiking the standards of PAHs with different concentrations into the soil or plant sample, and the recoveries of the 14 PAHs were 87.3–94.3% in soils and 85.2–93.5% in plant samples.

## Results and Discussion

**Root Uptake of PAHs.** Chemical compounds reach aerial plant organs in two ways: from the air and with the transpiration stream. Intensive studies were carried out to investigate the exchange of PAHs between air and leaves and their uptake from solution into plant stem and leaves (4, 20). The aim of this work was to thoroughly investigate PAH transport in the soil–root–shoot system. Therefore, PAH accumulation in plant roots and shoots using soil cultivation and shoot uptake of PAHs from the air using nonsoil control plants were determined. Concentrations of PAHs in roots are given in Table S3 in the Supporting Information. The concentrations of 2-, 3-, 4-, and 5–6-ring PAHs in roots correlated well with the corresponding concentrations in soils ( $n = 15$ ,  $r^2 = 0.603$ – $0.842$ ,  $p < 0.01$ ) (Figure S1 in the Supporting Information). The RCF was defined as the ratio of the PAH concentration in roots to that in soil on a dry weight basis (7). Log RCFs of the 14 PAHs were plotted against their log  $K_{ow}$ 's in Figure 1a. The average RCFs for 2-, 3-, 4-, and 5–6-ring PAHs were 6.91, 5.76, 8.28, and 1.46, respectively (slopes of the lines shown in Figure S1 in the Supporting Information). The 4-ring PAHs (Fla, Pyr, BaA, and Chr) showed higher RCF values than other PAHs, and Fla (log  $K_{ow} = 5.20$ ) showed the maximum RCF value among the 14 PAHs. The 5–6-ring PAHs (BbF, BkF, BaP, DahA, and BghiP, with log  $K_{ow}$  varying from 5.78 to 6.90) had the minimum RCF values. These results suggest that 4-ring PAHs had the highest tendency to be taken up by roots whereas 5–6-ring PAHs had the lowest likelihood of being taken up.



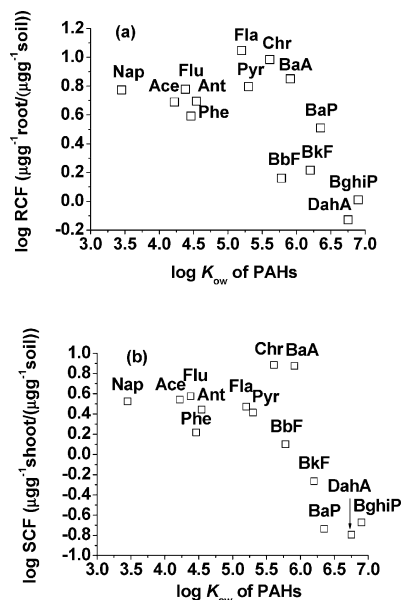


FIGURE 1. Relationship between RCF and shoot concentration factor (SCF) (on dry weight) and  $K_{ow}$  of PAHs.

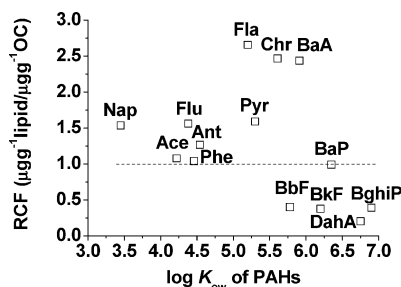


FIGURE 2. Normalized RCFs ( $\mu\text{g g}^{-1} \text{ lipid}/\mu\text{g g}^{-1} \text{ OC}$ ) of PAHs on the basis of root lipid and soil organic carbon.

Briggs et al. (6) found a positive linear relationship between log RCF and log  $K_{ow}$  in their experiments investigating the uptake of *O*-methylcarbamoylmines and substituted phenylureas by barley in hydroponic solution. Lin et al. (16) also observed a positive linear relationship between log RCF and log  $K_{ow}$  for the uptake of Nap, Ace, Flu, Phe, and Pyr by tea plants cultivated in hydroponic solution. However, in the present study no obvious linear relationship between log RCF and log  $K_{ow}$  for the 14 PAHs could be discerned. In hydroponic solution, PAHs only partitioned between roots and solution and their uptake by roots depended solely on the hydrophobicity of the compounds and root lipids. However, the situation becomes more complicated for plants grown in field-contaminated soils. In addition to being taken up by roots, there is a sorption-desorption equilibrium of PAHs on soil particles and in particular on soil organic matter (SOM). Therefore, the influence of all the factors involved such as properties of the organic compounds and plants, soil characteristics (particularly SOM), and pollution history needs to be considered. In the present study, a significant negative influence of soil organic carbon (SOC) content on the concentrations of 2-, 3-, 4-, 5-6-ring and the total concentration of the 14 PAHs in roots was found ( $p < 0.01$ ), suggesting an important role of SOM in the uptake of PAHs by roots from soil. Concentrations of PAHs in roots and soils were further normalized on root lipid and SOC basis, and the RCFs ( $\mu\text{g g}^{-1} \text{ lipid}/\mu\text{g g}^{-1} \text{ SOC}$ ) on the basis of root lipid and SOC are shown in Figure 2. After normalization, RCFs of 5-6-ring PAHs (BbF, BkF, BaP, DahA, and BghiP) were all lower than 1 and RCFs of other PAHs were all higher than 1. Four-ring PAHs (Fla, Pyr, BaA, and Chr) showed the highest

RCF values, which were in the range of 1.59–2.66. This result demonstrates that 5-6-ring PAHs have a lower affinity to root lipids than SOM, because of their extremely high hydrophobicity (with log  $K_{ow}$  varying from 6.20 to 6.90). Furthermore, after being desorbed into the soil solution highly hydrophobic compounds such as 5-6-ring PAHs diffuse very slowly into plant root tissue, so they are unlikely to reach equilibrium, and this results in a significant growth dilution (21, 22). In contrast, less hydrophobic compounds reach equilibrium or near-equilibrium diffusion into roots much more readily. Therefore, lower root concentration factors were obtained for the 5-6-ring PAHs in soils. There is degradation of PAHs in rhizosphere soil (23) and metabolism inside roots (15), and it probably occurred in this experiment although the soils were sterilized to reduce PAH degradation in soil to the minimum (24). Degradation of PAHs in soil was observed to vary from compound to compound and was more significant for lower-ring PAHs than higher-ring ones (23). Furthermore, different historical behavior of PAHs in field-contaminated soils should be considered. PAHs with lower molecular weight (e.g., 2-3-ring PAHs) have a much greater tendency to partition into the air and preferential degradation in soil. This can result in the loss of the bioavailable fraction of 2-3-ring PAHs and a lower RCF for 2-3-ring PAHs although the plants have the ability to draw these compounds to their roots by the transpiration stream much more readily. In contrast, PAHs with high molecular weight (e.g., 5-6-ring PAHs) are controlled by strong partitioning to soil, and as a consequence there is less opportunity for historical loss to the atmosphere and biodegradation. Nevertheless, because of their strong binding to soil, plants have less ability to draw these compounds to the roots by the transpiration stream, and therefore they also have lower RCF values.

**Accumulation of PAHs in Shoots.** Concentrations of PAHs in shoots are shown in Table S4 of the Supporting Information. Significant linear relationships were found between concentrations of 2-, 3-, 4-, and 5-6-ring PAHs or the total concentrations of the 14 PAHs in shoots and roots (Figure S2 in the Supporting Information). The average  $C_{\text{shoot}}/C_{\text{root}}$  ratios (slopes of the lines shown in Figure S2 in the Supporting Information) of 2-, 3-, 4-, and 5-6-ring PAHs were 0.57, 0.60, 0.56, and 1.79, respectively. The 5-6-ring PAHs had much higher  $C_{\text{shoot}}/C_{\text{root}}$  ratios than other PAHs, likely because of the more significant contribution of air-to-leaf transport of 5-6-ring PAHs to shoot accumulation due to their high partition coefficients between leaf and air. Concentrations of 2-, 3-, 4-, and 5-6-ring PAHs in wheat shoots were also found to correlate well with the corresponding concentrations in soils ( $n = 15$ ,  $r^2 = 0.640-0.820$ ,  $p < 0.01$ ) (Figure S3 in the Supporting Information). Shoot concentration factor, defined as the ratio of the PAH concentration in shoots to that in soil on a dry weight basis, was calculated (Figure 1b). The average SCFs of 2-, 3-, 4-, and 5-6-ring PAHs were 4.26, 4.31, 5.06, and 2.53, respectively (slopes of the lines shown in Figure S3 in the Supporting Information), and the 4-ring PAHs had the highest SCFs. The plot of log SCF against log  $K_{ow}$  is very similar to that of log RCF, implying root uptake of PAHs and subsequent translocation from roots to shoots may make a significant contribution to their accumulation in shoots. However, because of the high partition coefficients of PAHs, in particular for the 5-6-ring PAHs between leaf and air, a proportion of PAHs may also come from the air-to-leaf pathway. To clarify the possible dominant pathway for PAH uptake, distribution profiles of PAHs in soil, roots, shoots, and air were obtained as the PAHs with different rings expressed as a percentage of the total PAH concentrations. XAD-2 resin has been widely used as a passive sampler to sample and monitor PAHs in air (25). The percentage distribution of different PAHs in XAD-2 resin should be

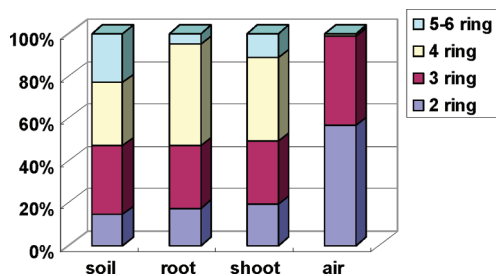


FIGURE 3. Percentage distribution profiles of PAHs in soils, roots, shoots, and air ( $n = 3$ ).

TABLE 1. Ratio of PAH from Root-to-Shoot Translocation to the PAH Concentration in Shoots ( $R_t$ , %)<sup>a</sup>

	Nap	Ace	Flu	Phe	Ant
$R_t$	$72.6 \pm 3.8$	$65.5 \pm 4.7$	$62.6 \pm 4.6$	$60.5 \pm 5.0$	$57.8 \pm 4.9$
	Fla	Pyr	BaA	Chr	BbF
$R_t$	$54.4 \pm 5.9$	$55.1 \pm 5.5$	$51.7 \pm 6.6$	$53.6 \pm 4.5$	$59.3 \pm 5.9$

<sup>a</sup>  $R_t = C_{\text{shoot,t}}/C_{\text{shoot}}$ .  $C_{\text{shoot,t}}$  is the concentration of PAH in shoots resulting from root-to-shoot translocation.

identical to that in the atmosphere. Therefore, the distribution profile of PAHs in XAD-2 resin was used to substitute for that in the air of the growth chamber. The results show that the distribution profiles were very similar for the 15 different soils. Therefore, the distribution profile for soil 5 was chosen and is displayed in Figure 3 as a typical example. The distribution of PAHs with different ring numbers in shoots was quite similar to that of the roots and soils but was significantly different from that of the atmosphere. The percentages of 2- and 3-ring PAHs were much lower in shoots than in air, whereas the percentages of 4- and 5–6-ring PAHs were much higher in shoots than in air. These results suggest that PAHs may be translocated from roots to shoots within wheat after being taken up by the roots.

**Acropetal Translocation of PAHs within Wheat.** To confirm whether the soil-to-plant pathway is the main route for PAH uptake by wheat, it is necessary to investigate the quantity of acropetal translocation of PAHs within the plants. PAHs in shoots are derived from two pathways: uptake from the atmosphere and translocation from roots. Therefore, PAH concentration in shoots resulting from root-to-shoot translocation from soil ( $C_{\text{shoot,t}}$ ) can be described by the following equation (16):

$$C_{\text{shoot,t}} = C_{\text{shoot}} - C_{\text{shoot,air}} \quad (1)$$

where  $C_{\text{shoot,air}}$  is the concentration of PAH uptake from air in the growth chamber, which can be substituted with the PAH concentration in shoots cultivated in hydroponic solution without addition of PAHs. The ratio of PAH from root-to-shoot translocation to the total accumulation in shoots ( $R_t$ ) can then be calculated by:

$$R_t = C_{\text{shoot,t}}/C_{\text{shoot}} \quad (2)$$

$R_t$  values are listed in Table 1. Translocation of Nap, Ace, Flu, Phe, Ant, Fla, Pyr, BaA, Chr, and BbF (in the  $\log K_{ow}$  range from 3.45 to 5.78) from roots to shoots was observed. Concentrations of more highly lipophilic PAHs (with  $\log K_{ow}$  varying from 6.20 to 6.90) were too low to be detected in shoots cultivated in hydroponic solution because of the very low concentrations of these compounds in air, and therefore their translocation is not discussed here. A significant negative linear relationship was found between  $\log R_t$  and  $\log K_{ow}$  of

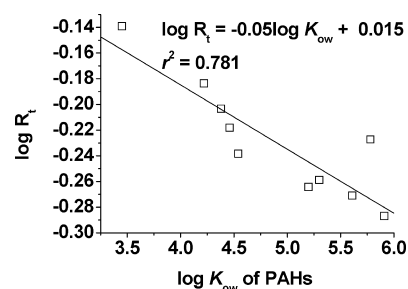


FIGURE 4. Relationship between  $\log R_t$  (ratio of PAH translocated from root-to-shoot to the total accumulation in shoots) and  $\log K_{ow}$  of PAHs.

the 10 PAHs (Figure 4), and the relationship can be expressed as:

$$\log R_t = -0.05 \log K_{ow} + 0.015 \quad (r^2 = 0.781, p < 0.01, n = 10) \quad (3)$$

Previous studies conducted with plants grown in hydroponic cultivation found that  $\log R_t$  for compounds with intermediate lipophilicity decreased with their increasing  $\log K_{ow}$  (16). But information on the quantitative relationship between  $\log R_t$  and  $\log K_{ow}$  of a series of HOCs with middle and high degrees of hydrophobicity has been rarely reported, particularly for the uptake of HOCs by plants grown in field-contaminated soils. In this study, a linear relationship between  $\log R_t$  and  $\log K_{ow}$  was found for 10 PAHs with  $\log K_{ow}$  and ranged from 3.45 to 5.78, which is consistent with the view that translocation of HOCs within the plant is associated with a series of chemical partitions between the plant aqueous phase and the organic components of the plant (4). More highly lipophilic PAHs have a higher tendency to partition and accumulate into organic constituents of the plants so that the fraction that can be drawn into the transpiration stream and be translocated within the plants is much lower, resulting in a lower root-to-shoot translocation.

## Acknowledgments

This work was funded by the National Natural Science Foundation of China (Projects 40730740 and 20621703) and the National Basic Research Program of China (No. 2009CB421603).

## Supporting Information Available

Sampling locations and the contents of TOC and DOC of the soils (Table S1), concentrations of PAHs in soils (Table S2), roots (Table S3), and shoots (Table S4), correlation of concentrations of PAHs in roots and soils (Figure S1), correlations between concentrations of PAHs in shoots and roots (Figure S2) and in shoots and soils (Figure S3). This material is available free of charge via the Internet at <http://pubs.acs.org>.

## Literature Cited

- (1) Fismes, J.; Perrin-Ganier, C.; Empereur-Bissonnet, P.; Morel, J. L. Soil-to-plant transfer and translocation of polycyclic aromatic hydrocarbons by vegetables grown on industrial contaminated soils. *J. Environ. Qual.* **2002**, *31*, 1649–1656.
- (2) McKone, T. E.; Madallena, R. L. Plant uptake of organic pollutants from soil: Biocentrations estimation based models and experiments. *Environ. Toxicol. Chem.* **2007**, *26*, 2494–2504.
- (3) Wild, S. R.; Jones, K. C. Polynuclear aromatic hydrocarbons uptake by carrots grown in sludge amended soil. *J. Environ. Qual.* **1992**, *21*, 217–225.
- (4) Collins, C.; Fryer, M.; Grosso, A. Plant uptake of non-ionic organic chemicals. *Environ. Sci. Technol.* **2006**, *40*, 45–52.
- (5) Simonich, S. L.; Hites, R. A. Organic pollutant accumulation in vegetation. *Environ. Sci. Technol.* **1995**, *29*, 2905–2914.

- (6) Briggs, G. G.; Bromilow, R. H.; Evans, A. A. Relations between lipophilicity and root uptake and translocation of non-ionised chemicals by barley. *Pestic. Sci.* **1982**, *13*, 495–504.
- (7) Hülster, A.; Müller, J. F.; Marschner, H. Soil-plant transfer polychlorinated dibenzo-*p*-dioxins and dibenzofurans to vegetables of the cucumber family (Cucurbitaceae). *Environ. Sci. Technol.* **1994**, *28*, 1110–1115.
- (8) White, J. C. Plant-facilitated mobilization and translocation of weathered 2,2'-bis(*p*-chlorophenyl)-1,1'-dichloroethylene (*p,p'*-DDE) from an agricultural soil. *Environ. Toxicol. Chem.* **2001**, *20*, 2047–2052.
- (9) Mattina, M. J.; Berger, W. I.; Dykas, L. Chlordane uptake and its translocation in food crops. *J. Agric. Food Chem.* **2000**, *48*, 1909–1915.
- (10) Lee, W. Y.; Iannucci-Berger, W. A.; Eitzer, B. D.; White, J. C.; Mattina, M. J. I. Plant uptake and translocation of airborne chlordane and comparison with the soil-to-plant route. *Chemosphere* **2003**, *53*, 111–121.
- (11) Kipopoulou, A. M.; Manoli, E.; Samara, C. Bioconcentration of polyaromatic hydrocarbons in vegetables grown in an industrial area. *Environ. Pollut.* **1999**, *106*, 369–380.
- (12) Gao, Y.; Zhu, L. Plant uptake, accumulation and translocation of phenanthrene and pyrene in soils. *Chemosphere* **2004**, *55*, 1169–1178.
- (13) Wild, E.; Jones, K. C. Seeing chemicals in environmental samples. *Environ. Sci. Technol.* **2007**, *41*, 5935–5938.
- (14) Wild, E.; Dent, J.; Thomas, G. O.; Jones, K. C. Direct observation of organic contaminant uptake, storage, and metabolism within plant roots. *Environ. Sci. Technol.* **2005**, *39*, 3695–3702.
- (15) Wild, E.; Dent, J.; Barber, J. L.; Thomas, G. O.; Jones, K. C. A novel analytical approach for visualizing and tracking organic chemicals in plants. *Environ. Sci. Technol.* **2004**, *38*, 4195–4199.
- (16) Lin, D. H.; Zhu, L. Z.; He, W.; Tu, Y. Y. Tea plant uptake and translocation of polycyclic aromatic hydrocarbons from water and around air. *J. Agric. Food Chem.* **2006**, *54*, 3658–3662.
- (17) Liu, S.; Tao, S.; Liu, W.; Dou, H.; Liu, Y.; Zhao, J.; Little, M. J.; Tian, Z.; Wang, J.; Wang, L.; Gao, Y. Seasonal and spatial occurrence and distribution of atmospheric polyaromatic hydrocarbon (PAHs) in rural and urban areas of the North Chinese plain. *Environ. Pollut.* **2008**, *156*, 651–656.
- (18) Nelson, D. W.; Sommers, L. E. Total carbon, organic carbon and organic matter. In *Methods of Soil Analysis, Part 2*; Page, A. L., Ed.; American Society of Agronomy: Madison, WI, 1982.
- (19) Li, H.; Sheng, G.; Chiou, C.; Xu, O. Relation of organic contaminant equilibrium sorption and kinetic uptake in plant. *Environ. Sci. Technol.* **2005**, *39*, 4864–4870.
- (20) Trapp, S.; McFarlane, J. C. *Plant Contamination: Modeling and Simulation of Organic Chemical Processes*; Lewis Publishers: Boca Raton, FL, 1995.
- (21) Trapp, S. Dynamic root uptake model for neutral lipophilic organics. *Environ. Toxicol. Chem.* **2002**, *21*, 203–206.
- (22) Trapp, S.; Cammarano, A.; Capri, E.; Reichenberg, F.; Mayer, P. Diffusion of PAH in potato and carrot slices and application for a potato model. *Environ. Sci. Technol.* **2007**, *41*, 3103–3108.
- (23) Rezek, J.; Wiesche, C.; Mackova, M.; Zadrzil, F.; Macek, T. The effect of ryegrass (*Lolium perenne*) on decrease of PAH content in long term contaminated soil. *Chemosphere* **2008**, *70*, 1603–1608.
- (24) Wang, J. Y.; Yang, L.; Tseng, C.; Hsu, H. Application of phytoremediation on soil contaminated by pyrene. *Environ. Eng. Sci.* **2008**, *25*, 829–838.
- (25) Wei, M.; Chang, W.; Jen, J. Monitoring of PAHs in air by collection XAD-2 adsorbent then microwave-assisted thermal desorption coupled with head solid-phase microextraction and gas chromatography with mass spectrometric detection. *Anal. Bioanal. Chem.* **2007**, *387*, 999–1005.

ES803368Y