Environ. Sci. Technol. 43, 9136–9141

Partitioning of Phenanthrene by Root Cell Walls and Cell Wall Fractions of Wheat (*Triticum aestivum* L.)

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Received July 13, 2009. Revised manuscript received October 29, 2009. Accepted November 3, 2009.

Plant cells have been reported to play an important role in the uptake of organic contaminants. This study was undertaken to provide an insight into the role of the root cell walls and their subfractions on sorption of phenanthrene to roots of wheat (*Triticum aestivum* L.). Root cell walls were isolated and further sequentially fractioned by removing pectin, hemicellulose one, and hemicellulose two. They were characterized by elemental analysis, Fourier transform infrared spectroscopy, and solid-state ^{13}C NMR. Root cell walls had a greater proportion of aromatic carbon and exhibited a lower polarity than the bulk roots. There was a stepwise increase in aromatic carbon content and a decrease in polarity following the sequential fractionation. The sorption affinity of phenanthrene increased gradually following the sequential extraction of root cells. A significant positive correlation between the sorption affinity K_{OC} values and the aromatic carbon contents ($r^2 = 0.896$, $p < 0.01$) and a negative correlation between the sorption affinity K_{OC} values and polarity ((O + N)/C) of root cell fractions ($r^2 = 0.920$, $p < 0.01$) were obtained. Improved modeling was achieved for phenanthrene sorption by involving the contribution of root cell walls as a source of root carbohydrates instead of using root lipids alone, which further confirms the significant contribution of root cell walls to phenanthrene sorption on wheat roots. The results provide evidence for the importance of the root cell walls in the partitioning of phenanthrene by plant roots.

Introduction

Plant uptake of organic contaminants is an important process when considering the risks associated with land contamination, the role of vegetation in the global cycling of persistent organic pollutants, and the potential for industrial discharges to contaminate the food chain. Organic contaminants may enter a plant via both root uptake (*1*−*3*) and foliar uptake (*4, 5*) and are then translocated to other parts of the plant. Root uptake is usually predominant over foliar uptake for hydrophobic organic compounds (HOCs) of low volatility (*6*). An improved understanding of root uptake and subsequent accumulation and translocation of HOCs inside plants will have considerable benefits for risk assessment associated with soil contamination and control of food contamination (*7*).

Using two-photon excitation microscopy coupled with autofluorescence (TPEM-AF), Wild and his co-workers (*8, 9*) have investigated the uptake and movement of the polycyclic aromatic hydrocarbons (PAHs) phenanthrene and anthracene inside living plant roots. There is evidence that apoplastic movement can occur through both cell walls and intercellular spaces but not entry into the cells. Symplastic movement can occur through cell cytoplasm and plasmodesmata or transcellularly across cell membranes. Both translocation pathways provide opportunities for organic contaminants to make contact with the cell wall. Therefore, partitioning of HOCs such as PAHs to the cell wall may be an important process during their uptake and transfer in plants.

The presence of a complex and dynamic cell wall is one of the most important distinguishing features of plant cells. The cell wall is the outermost surface of a cell and is composed mostly of cellulose, a complex carbohydrate made up of several thousand glucose molecules linked end-to-end, two groups of branched polysaccharides, pectins and cross-linking glycans, highly glycosylated proteins, and lignin (*10*). As the first line of defense against environmental threats, plant cell walls control the transport of molecules into the cells and may also provide functions affecting the transpiration and translocation of pollutants in plants. Therefore, elucidation of the fundamental functions of the plant cell wall in the interactions between root cell walls and organic contaminants is of great importance. However, a thorough understanding of the role of root cell walls in the partitioning and uptake of HOCs is still lacking.

Plant uptake of HOCs can be considered as a series of local partition processes between various plant organic components and water (or soil-water). On the basis of this, a partition-limited plant uptake model was formulated (*11*) and tested in some plant species with satisfactory results (*6, 12, 13*). The model analysis indicated that the plant lipid content was predominant for the sorption or uptake of HOCs and therefore the partition-limited model was further simplified into a lipid model (*6*). However, later studies found that sorption of organic contaminants by plant roots estimated by the lipid model was much lower than the measured data for contaminants such as phenanthrene (*12, 14*), lindane and hexachlorobenzene (*6*), and benzene and 1,2-dichlorobenzene (*12*). Recent research by Zhang and Zhu (*15*) suggested that the contribution of carbohydrates to sorption or uptake of organic contaminants should not be neglected. Cell walls, in particular the thick and strong secondary walls, account for most of the carbohydrates in root biomass. Therefore, we hypothesized that if plant carbohydrate components make a contribution to plant uptake of HOCs, this might primarily contribute to the role of the root cell walls. Therefore, a test of the partition-limited model for plant uptake of HOCs by considering root cell walls as a source of root carbohydrates is necessary.

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10.1021/es902098p
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Published on Web 11/18/2009

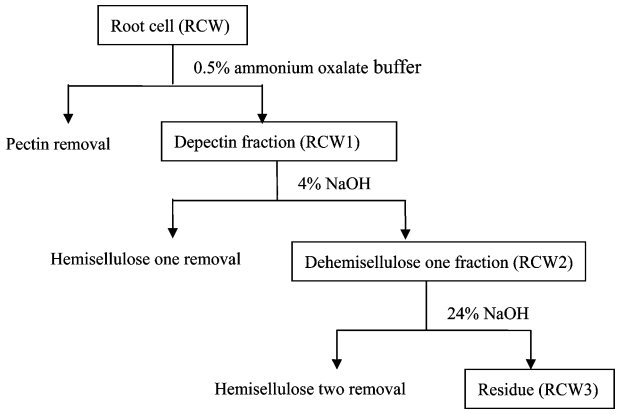

FIGURE 1. Flowchart of the isolation process of cell wall fractions.

The present study was carried out with two purposes. The first was to elucidate the conformational and sorptive characteristics of root cell walls and cell wall individual components. Sorption of phenanthrene as a model HOC on wheat roots, root cell walls, and cell wall subfractions was quantitatively evaluated and the subfractions were characterized by elemental analysis, Fourier transform infrared spectroscopy, and solid-state ^{13}C NMR. The second purpose was to compare modeling of root partitioning of phenanthrene using root lipids either alone or together with root cell walls as a source of root carbohydrates in order to elucidate the contribution of carbohydrates to root uptake of phenanthrene to provide further evidence for the important role of root cell walls in HOC uptake by plants.

Materials and Methods

Preparation of Roots, Root Cell Walls, And Their Fractions. Wheat (*Triticum aestivum* L.) was used as the test plant and was separated into roots and shoots, blotted dry with tissue paper, and immediately weighed. The root samples were then frozen at −80 °C overnight, freeze-dried for 48 h in a lyophilizer (FD-1, Beijing Boyikang Instruments Ltd.), and weighed. The dried root samples were then ground separately and sieved (<0.25 mm). Determination of root lipid content followed the same principles as employed previously in our laboratory (*14*). The details are supplied in the Supporting Information. Root cell walls were obtained by extraction with ice-cold (−18 °C) 75% ethanol and kept undisturbed for 20 min in an ice−water bath. Afterward, they were further fractionated according to the procedure described in Figure 1 and three subfractions were obtained. The details of the extraction and sequential fractionation of the cell walls are provided in the Supporting Information.

Characterization of Roots, Root Cell Walls, And Their Fractions. The elemental composition (C, H, and N) was analyzed by a high-temperature combustion method (PE 2400 Series II Analyzer, Pekin-Elmer, Inc.). Ash content was determined by combustion of the samples at 740 °C for 4 h. The contents of all of the elements were calculated on an ash-free basis. Oxygen content was calculated by the mass difference. The mass atomic ratios, H/C, O/C and (N + O)/C of the sorbents, were calculated by their elemental composition and atomic weights.

Infrared spectra were acquired on a Nexus 670 Fourier transform infrared (FTIR) spectroscope (Thermo Nicolet Company, Madison, WI) equipped with deuterated triglycine (DTGS) and mercury−cadmium−telluride (MCT) detectors (Thermo Nicolet Company), a KBr beam splitter (Thermo Nicolet Company) and a sample bench purged with dry air. The resolution of FTIR spectroscopy was 2.0 cm^{-1}, and a total of 64 scans were collected for each spectrum. The samples were freeze-dried overnight. The FTIR spectra of pellets of a mixture of 1.5 mg of sample and 100 mg of dried KBr pressed under reduced pressure were recorded.

Solid-state ^{13}C NMR data were acquired using cross-polarization and magic angle spinning (CPMAS) on a 300-MHz NMR spectrometer (Varian, San Francisco, CA). The instrument was run under the following conditions: contact time, 1 ms; spinning speed, 5 kHz; 90° H pulse, 5 μs; acquisition delay, 4 s; line broadening, 50 Hz; and number of scans, 2000−5000.

Batch Sorption Experiment. Phenanthrene was purchased from Acros Organics (Morris Plains, NJ) with a labeled purity of >99% and used as received. The aqueous solubility of phenanthrene at 22 °C is 1.12 mg/L, and log K_{OW} is 4.46 (*16*). Phenanthrene stock solution was prepared in high-performance liquid chromatography (HPLC)-grade methanol due to its low aqueous solubility. The working solution was prepared by diluting the stock solution with background solution and methanol concentrations in the final solutions were always kept below 0.1% (v/v) to minimize cosolvent effects.

Sorption of phenanthrene by freeze-dried roots, root cell walls, and cell wall fractions was studied using a batch equilibration technique in triplicate. A series of phenanthrene solutions with a range of initial concentrations (0.05−1.00 mg L^{-1}) were prepared using half-strength Hoagland solution as the matrix and with 200 mg L^{-1} NaN_3 as a biocide. Subsamples of 5 mg of dry plant material (roots, root cell walls, or cell wall fractions) and 20 mL phenanthrene solution were combined in 40 mL glass centrifuge tubes with Teflon-lined caps. The solid-to-liquid ratios were chosen to allow 30−80% of the added solute to be sorbed at equilibrium. Controls were prepared for each isotherm experiment for quality assurance. Blank controls contained solute and water but no plant material and were used to measure any phenanthrene losses. Recoveries from blanks were, on average, 96%, suggesting that the losses of phenanthrene by evaporation, degradation, and sorption to the glass vials during the experiment were negligible. Background controls contained plant material and water but no solute and were used to detect any contamination. The tubes were shaken for 48 h on a tumble shaker at 100 rpm at 20 ± 1 °C (previous kinetic measurements indicated that apparent equilibrium was reached before 24 h). Following the equilibration and subsequent 30 min sedimentation of plant materials, the vials were centrifuged at 1000 × *g* for 30 min and the supernatant from each tube was analyzed for solute. The phenanthrene concentration in the plant was calculated from the difference between the initial and final concentrations in the water phase because the loss of solute by processes other than sorption was found to be less than 5%. The standard deviation of six replicate determinations of phenanthrene standard solution at a concentration of 1.00 mg L^{-1} was 1.6% after 72 h of shaking. Phenanthrene concentration was analyzed by HPLC (Agilent 1200 series) equipped with an ultraviolet detector using a reverse-phase C_{18} column (4.6 × 150 mm, 5 μm particle size). Details of the instrumental conditions were the same as those used in previous work (*1*). Data were analyzed using the Origin 7.0 software.

The Sorption Model. Plant sorption of phenanthrene from water can be described as follows (*6*):

$$\text{the sorption model: } Q_{eq} = C_w K_{pl} \quad (1)$$

$$\text{the composition model: } Q_{eq} = C_w(f_{lip}K_{lip} + f_{ch}K_{ch}) \quad (2)$$

$$\text{the lipid model: } Q_{eq} = C_w(f_{lip}K_{lip}) \approx C_w f_{lip}K_{ow} \quad (3)$$

where Q_{eq} is the concentration of solute in the plant (mg of contaminant/kg of plant material) at equilibrium. C_w is the concentration of solute in water (mg of contaminant/kg of

TABLE 1. Integration Results of Elemental Composition and Solid-State ^{13}C NMR Spectra[a]

sample	C (%)	H (%)	O (%)	N (%)	ash (%)	H/C	O/C	(O+N)/C	distribution of C chemical shift (ppm) (%) 0−45	45−90	90−114	114−140	140−165	140−165	190−220	aliphatic C (%)	aromatic C (%)	polar C (%)
roots	38.69	5.59	44.11	1.16	10.45	1.734	0.855	0.881	5.1	71.7	14.2	1.1	2.9	3.0	2.0	91.0	4.0	93.8
RCW	41.24	5.79	40.84	1.11	11.02	1.685	0.743	0.766	5.3	71.9	13.5	2.2	3.2	2.1	1.9	90.8	5.3	92.6
RCW1	41.43	5.83	39.33	0.88	12.53	1.689	0.712	0.730	5.5	63.6	11.1	4.9	5.0	6.4	3.5	80.1	10.0	89.6
RCW2	40.96	6.23	38.48	0.58	13.75	1.825	0.705	0.717	6.4	61.0	8.9	5.4	5.7	7.2	5.4	76.3	11.1	88.2
RCW3	41.56	6.37	37.42	0.46	14.19	1.839	0.675	0.685	11.7	51.4	7.5	10.6	6.9	7.6	4.2	70.7	17.5	77.7

[a] Aliphatic C: total aliphatic carbon region (0−114 ppm); Aromatic C: total aromatic carbon region (114−165 ppm); Total polar C region (45−114 and 140−220 ppm).

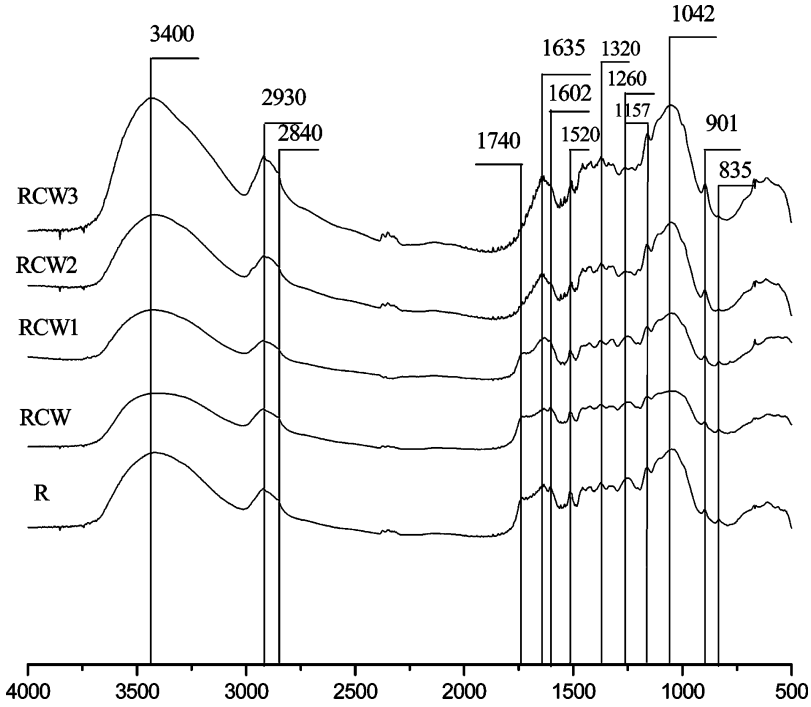

FIGURE 2. Fourier transform infrared spectra of wheat roots (R), wheat root cell walls (RCW) and wheat root cell wall fractions (RCW1, RCW2, and RCW3).

water) at equilibrium. In eq 1 the ratio Q_{eq}/C_w (K_{pl}) is equivalent to the slope of the corresponding sorption isotherm. f_{lip} and f_{ch} are the respective weight fractions of root lipids and root cell walls, and K_{lip} and K_{ch} are the root lipid−water partition coefficient and the root cell wall-water partition coefficient of the solute, respectively.

Results and Discussion

Characterization of Root, Root Cell Wall, And Cell Wall Fractions. The relative yield and elemental compositions of wheat roots, root cell walls, and cell wall fractions are listed in Table 1. Cell wall dry weight accounted for 82.7% of the root dry mass. The residual fraction with the removal of pectin and hemisellulose was still 24.3% of the bulk root mass. After root cell wall extraction in which membranes and adhering proteins were dislodged, the lipid contents were reduced from 3.01% for bulk roots to 0.9% for root cell walls. The H/C ratios of all of the root materials were in the range of 1.685−1.839, exhibiting a highly aliphatic nature. Root cell walls had a higher C content and lower O and N contents than the bulk roots, and thus lower polarity. The polarity index ((O + N)/C) decreased gradually with the sequential fractionation of root cell walls, which is consistent with the removal of polar organic functions such as the carboxylic acid moiety in hemicelluloses as a result of extraction with sodium hydroxide.

Characterization was conducted by FTIR spectroscopy (Figure 2). All five spectra appear to be similar. However, on closer examination a gradual disappearance of the absorption at 1740 cm^{-1} is apparent, arising mainly from the carboxylic or carbonyl C═O linkage in acetyl ester groups from hemicellulose (*17, 18*). This is consistent with the decomposition of hemicellulose following sequential fractionation of root cell walls. There is a decrease in the relative absorbance at 1520 cm^{-1} assigned to N−H deformation or C═N stretching or aromatic C═C stretching, in good agreement with the elemental analysis results (Table 1) in which the percent composition of nitrogen declined following cell wall isolation and fractionation.

Cell wall materials were further characterized by solid-state ^{13}C NMR spectroscopy and the spectra are shown in Figure 3 and the integration results are summarized in Table 1. The spectra were integrated as follows: alkyl-C (0 − 45 ppm); O-alkyl-C (45 − 114 ppm); aromatic-C (114 − 165 ppm); carboxylic- and amide-C (165 − 190 ppm) (*19*). Spectral results show dominating signals in the chemical shift region 45 to 114 ppm, indicative of O-alkyl, the most primary constituent of hemicellulose and polysaccharides in cellulose of root cell walls as well as methoxyl groups in lignin (*20, 21*). There is a clear decline in the levels of O-alkyl C following sequential fractionation as a result of the removal of hemicellulose by extraction. Isolation of root cell walls in which membranes and adhering proteins were dislodged did not reduce, but slightly increased, the percentage of aromatic carbon from 4.0% in roots to 5.3% in root cell walls, and the fraction of aromatic carbon (114−165 ppm) was

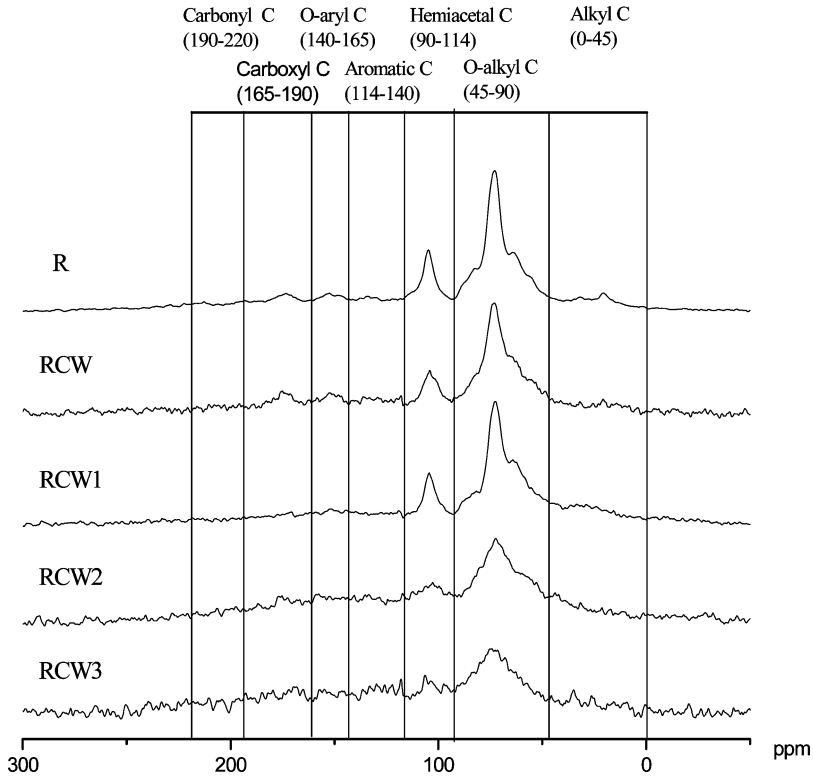

FIGURE 3. Solid-state ^{13}C NMR spectra of wheat roots (R), wheat root cell walls (RCW) and wheat root cell wall fractions (RCW1, RCW2, and RCW3).

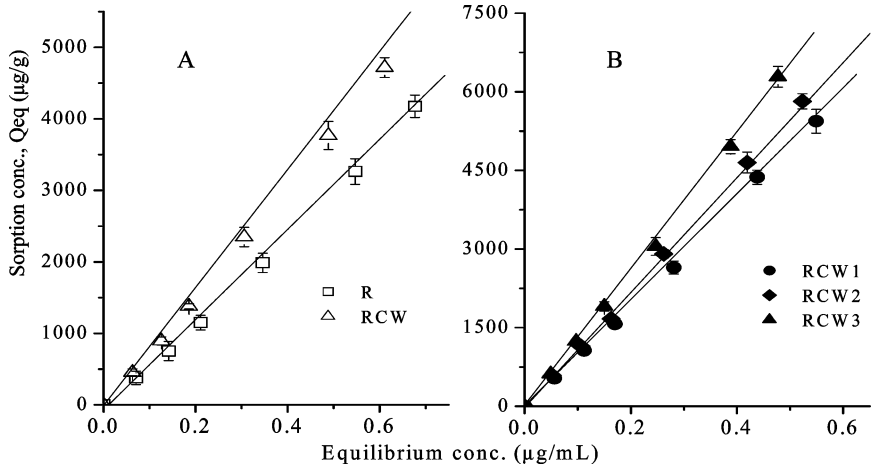

FIGURE 4. Sorption of phenanthrene by (A) wheat roots and root cell walls, and (B) root cell wall fractions on dry weight basis.

enhanced gradually from 5.3% for RCW to 17.5% for RCW3 and the fraction of the polar carbon (45−114 and 140−220 ppm) was reduced, indicating a gradual increase in aromaticity and decrease in polarity following the sequential fractionation of root cell walls.

Sorption of Phenanthrene to Wheat Root, Wheat Root Cell Walls, And Their Subfractions. Sorption of phenanthrene to wheat roots, wheat root cell walls and their fractions is displayed in Figure 4. The sorption isotherms are highly linear (r^2 values from 0.9967 to 0.9994), characteristic of a partition-dominated process. The partition coefficients (K_{OC}) of phenanthrene were obtained from the slopes of the corresponding sorption isotherms and normalized on carbon contents and were 5991.7, 7680.0, 9846.5, 11059.5, and 12873.1 mL/g for roots, root cell walls and cell wall fractions, respectively. Details for the sorption isotherms are given in Table S1 of the Supporting Information. In comparison, the root cell walls have a stronger partition for phenanthrene than the bulk roots, and a gradual increase in the sorption affinity was observed after each fractionation of root cell walls.

The composition and physicochemical nature of sorbents play an important role in the sorption of organic pollutants to natural sorbents (*22*). According to the above characterization results, root cell walls exhibit a lower polarity and a higher aromaticity than the bulk roots, which would favor the sorption of HOCs. This is consistent with the observation that root cell walls had a higher sorption capacity for phenanthrene than the bulk roots. Sequential fractionation of root cell walls led to a stepwise increase in aromatic carbon content and a decrease in polar carbon, and subsequently a gradually enhanced sorption affinity for phenanthrene. The relationships between sorption coefficients (K_{OC}) and aromatic carbon content and polarity of the root materials were further plotted. A strong positive correlation ($r^2 = 0.896$, $p < 0.01$) between K_{OC} values and the aromatic carbon contents

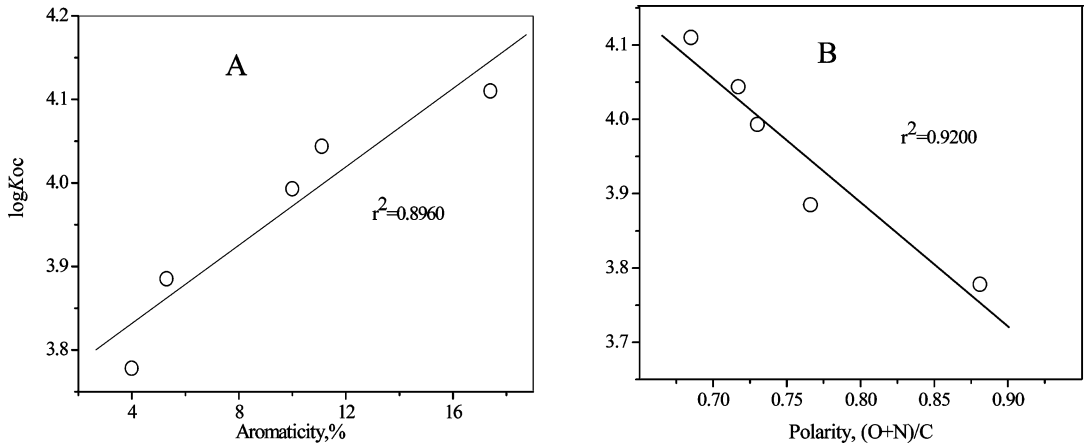

FIGURE 5. Relationship between sorption coefficients K_{OC} of phenanthrene and (A) aromatic carbon content and (B) polarity of the root materials.

(Figure 5A) was observed, which is consistent with the common hypothesis that an increase in the aromaticity of a sorbent results in an increase in the sorption of nonionic organic contaminants (*22*). Further, fractionation destroyed some of the hydrogen bonds and modified the structure and configuration of the cell wall fractions (*18*) resulting in the easy access of PAH to the aromatic cores, which increased the K_{OC} in comparison with that of the bulk roots and gradually with sequential fractionation of root cell walls. In addition to aromatic moieties, the polarity of a sorbent can significantly affect the sorption capacity of HOCs (*23, 24*). A negative correlation was observed between K_{OC} and the polarity index ((O + N)/C)) for root cell wall and cell wall fractions (Figure 5B, $r^2 = 0.920$, $p < 0.01$), which is consistent with previous reports (*23*−*26*).

Improved Estimation of Phenanthrene Sorption to Roots by Including Contribution of Root Cell Walls. Except for water, plant components can be categorized into plant lipids and carbohydrates (*11*). The plant lipid fraction is considered to be the main storage site of HOCs and therefore the predominant site for the sorption or uptake of HOCs by plants. However, the role of carbohydrate materials in sorption has been generally underestimated, even though carbohydrate components make up a significant portion of the composition of plants. Some recent studies have shown an underestimated sorption for HOCs by using plant lipid alone (*6, 12, 14, 15*). The most abundant component of the root cell wall is the carbohydrate cellulose. Therefore, if the carbohydrate fraction makes a contribution to the sorption of HOCs to roots, we may speculate that this is attributable to the role of root cell walls. To address this question, sorption of phenanthrene was estimated by the composition model in eq 2 with root lipid and root cell walls as the source of root carbohydrates. In the equation, the weight fractions of root lipids and root cell walls f_{lip} and f_{ch} are known; root cell wall−water partition coefficient K_{ch} can be obtained from the sorption isotherm for phenanthrene by root cell walls; and the root lipid−water partition coefficient K_{lip} can use the respective K_{ow} value since octanol is known to mimic biological lipids closely in contaminant partition (*11*). An excellent estimation was achieved as shown in Figure 6. In comparison, modeling with lipid alone using the lipid model in eq 3 provided a notably lower predicted sorption of phenanthrene than the measured values. This result provides further evidence for the significant contribution of root cell walls to the uptake of phenanthrene as well as the role of root cell walls as the carbohydrate pool of roots. In a recent study by Zhang and Zhu (*15*), an affinity of PAHs for carbohydrates of ryegrass roots was also observed that was extremely close to the affinity for the cell wall.

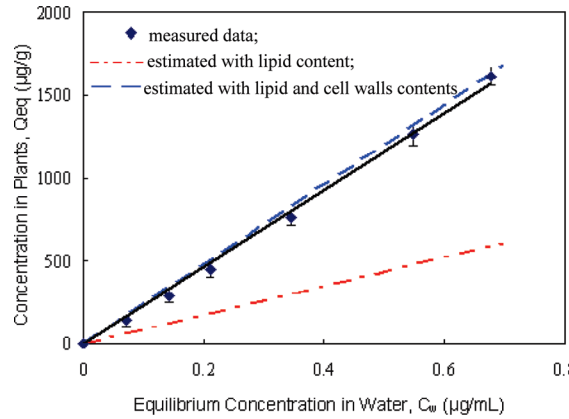

FIGURE 6. Sorption of phenanthrene by wheat roots on dry weight basis: experimentally determined vs modeled with root lipid and root cell walls.

This study characterizes for the first time the sorption of phenanthrene on plant root cell walls and their subfractions. Root cell walls have a stronger sorption affinity for phenanthrene than the bulk roots, and a gradual increase in the sorption affinity was observed after each sequential extraction of root cell walls. Furthermore, elemental composition analysis, FTIR spectroscopy and solid-state ^{13}C NMR provide convincing explanations for the discrepancy of sorption behaviors. Although mainly composed of carbohydrates, root cell walls make a significant contribution to the sorption of phenanthrene to roots. Therefore, integral roles of different plant constituents on the partition of HOCs should be considered for an accurate understanding of the uptake of organic contaminants by plants.

Acknowledgments

This work was funded by the National Natural Science Foundation of China (Projects 40730740, 20877083 and 20621703) and the National Basic Research Program of China (Project 2009CB421603).

Supporting Information Available

The methods used for determination of root lipid content, root cell wall extraction and sequential fractionation, and the sorption isotherms for phenanthrene (Table S1) are provided. This information is available free of charge via the Internet at http://pubs.acs.org.

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ES902098P