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Diffusion of PAH in Potato and Carrot Slices and Application for a Potato Model

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A method for quantifying the effect of medium composition on the diffusive mass transfer of hydrophobic organic chemicals through thin layers was applied to plant tissue. The method employs two silicone disks, one serving as source and one as sink for a series of PAHs diffusing through thin layers of water, potato tissue, and carrot tissue. Naphthalene, phenanthrene, anthracene, and fluoranthene served as model substances. Their transfer from source to sink disk was measured by HPLC to determine a velocity rate constant proportional to the diffusive conductivity. The diffusive flux through the plant tissue was modeled using Fick's first law of diffusion. Both the experimental results and the model suggest that mass transfer through plant tissue occurs predominantly through pore water and that, therefore, the mass transfer ratio between plant tissue and water is independent of the hydrophobicity of the chemical. The findings of this study provide a convenient method to estimate the diffusion of nonvolatile organic chemicals through various plant materials. The application to a radial diffusion model suggests that "growth dilution" renders the concentration of highly hydrophobic chemicals in potatoes below their equilibrium partitioning level. This is in agreement with field results for the bioconcentration of PAHs in potatoes.

Introduction

Potato is the fourth most important food crop in the world after wheat, rice and maize (*1*). The average daily consumption of potatoes and potato products in Denmark is 126 g, which is 58% of fruit and vegetable consumption (*2*). The situation is likely to be similar for many other countries, making potatoes the most important vegetable worldwide.

Botanically, potato is a tuber and, as such, is a part of the stem (*1*). It is not connected to the root system and the transpiration stream. It is loaded via phloem from the leaves. For hydrophobic organic compounds, translocation downward in phloem is negligible (*3*). The uptake of hydrophobic organic contaminants into potatoes is, therefore, most likely to occur from soil and via diffusion through the peel.

Diffusive mass transfer of chemicals in a multimedia-multiphase environment can involve the gas phase, aqueous phase, lipid phase, organic matter, and various solid inorganic phases. One way to approach such multimedia mass transfer are models that combine phase partitioning and Fick's first law of diffusion. This requires knowledge of the diffusion coefficients and the partition coefficients within and between the various phases (*4*). Their determination requires considerable experimental effort, and the resulting equations for the prediction of transport can be complex. Another way to approach the diffusive transfer of a chemical in multiphase systems is the determination of the diffusive conductivity, integrating diffusion, binding, and partitioning. An experimental method to quantify the effect of medium composition on the diffusive conductivity for hydrophobic organic chemicals was recently described (*5*). The method employs two poly(dimethylsiloxane) (PDMS) silicone disks, one serving as source and the other as sink for hydrophobic organic chemicals diffusing through thin layers. In the present study we modified this method to make it applicable to thin slices of plant tissue. The method was then used to determine the diffusive mass transfer of four PAHs through thin slices of potato and carrot. The experimental results were compared to the theory to develop a model for diffusive uptake of organic chemicals from soil into potatoes. The model was compared to field observations to validate the method.

Materials and Methods

Experimental Methods. Poly(dimethylsiloxane) (PDMS) sheets with a thickness of 600 μm ($\pm$20 μm) were supplied by Rubber BV. Sodemann Industrifjedre A/S (Viby, Denmark) supplied 100-μm steel washers (ID 4 mm, OD 8 mm) to be used as spacers for the water experiments. Nickel-plated neodymium iron boron magnets with a diameter of 10 mm and a thickness of 5 mm were supplied by Farnell (Herlev, Denmark). Naphthalene (NAP, >99%, Sigma), phenanthrene (PHT, >96%, Sigma), anthracene (ANT, 97%, Aldrich), and fluoranthene (FLT, >97%, Fluka) were supplied by Sigma-Aldrich (Vallensbæk Strand, Denmark). The PAHs were extracted from the PDMS disks with 96% ethanol (De Danske Spritfabrikker, Aalborg, Denmark).

Preparation of Thin Slices. Carrots (*Daucus carota* L. ssp. *sativus*) and potatoes (*Solanum tuberosum* L.) were purchased from a local supermarket. The carrots were purchased with green tops in order to ensure a fresh product. Potatoes were also selected for freshness. A large number of carrot and potato slices were cut using an electric ham slicer (model Euro 2560S from Graef, Arnsberg, Germany). The slice thickness was measured using a digital micrometer with a resolution of 10 μm. Slices with a thickness between 90 and 110 μm were selected. Circles with a diameter of 6 mm were cut from these slices and stored at 100% humidity.

Experimental Apparatus. Disks with a diameter of 6 mm were cut out of the PDMS sheet and cleaned in three changes of >200 mL methanol with a total contact time of at least 24 h. Disks were contaminated according to ref *6* by placing them in a methanol:water solution (80:20, v/v) containing the PAHs at a concentration of 0.5 mmol/L each, with a minimum contact time of 16 h. The homogeneous distribution of PAHs within the PDMS has been previously demonstrated (*7*). On the day of the experiment, contaminated disks were transferred to a small volume of water ($\cong$1 mL/disk) to remove methanol.

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Microchambers (Figure in Supporting Information or ref *5*) for the measurement of mass transfer by partitioning-diffusion-partitioning were assembled by placing the thin plant slices between a contaminated PDMS disk (the source) and a clean PDMS disk (the sink). For the water measurements, the two disks were separated by inserting a steel washer with a thickness of 100 μm, which served as a circular spacer and as a gasket for keeping the water in place. The whole microchamber was conveniently assembled on a horizontal glass plate with steel backing and pressed together using a magnet. Within the microchamber, PAH molecules partitioned from the source disk into the matrix, diffused through the 100-μm plant slice (or water), and finally partitioned into the sink disk. Measurements were terminated by removing the magnet and transferring each disk into 0.3−2 mL of ethanol for extraction of the PAHs. Measurements were performed in triplicate and with termination times between 15 min and 50 h. All experiments were conducted at room temperature (23 ± 3 °C).

Analytical Procedure. Ethanol extracts were analyzed for PAHs using HPLC with fluorescence detection (Agilent 1100 system with G1321A FLD (Ex. 260 nm; Em. 350, 420, 440, and 500 nm)). The separation column "CP-Ecospher 4 PAH" obtained from Varian Inc. (Palo Alto, CA) was operated at 0.5 mL/min (28 °C, 10 μL injection). Methanol (HPLC grade from Merck Darmstadt, Germany) and water (SUPER-Q treated, Millipore, MA) was used as mobile phase: 80% methanol at t = 0−5 min, linear gradient from 80 to 90% methanol at t = 5−10 min and from 90 to 100% methanol at t = 10−12 min. PAH concentrations in the extracts were quantified using a five-point external standard curve. Analysis was generally carried out within two weeks post sampling. Signal integration was performed with HP Chemstation software (A.06.03, Agilent Technologies, Palo Alto, CA) and corrected by hand as necessary.

Generally, 90−110% of initial concentrations of PAHs were recovered in the final extracts of sink and source disks, indicating a complete mass balance. The final time points of each time series were removed, partly due to decreasing mass balances and partly because it appeared difficult to maintain a stable tissue slice and water layer for more than 15−25 h. For naphthalene, we had to accept recoveries down to 80% to obtain sufficient data sets. Finally, the percentage that was transferred to the sink disk (T_{sink}) was fitted for each PAH with the equation

$$T_{Sink} = 50\% \times (1 - e^{-kt}) \quad (1)$$

to determine the velocity rate constant k. All nonlinear regressions were performed using GraphPad Prizm 4 (San Diego, California) by least-squares.

Measurement Endpoints. The velocity rate constant, k, describes the kinetics of the system and may, for instance, be used to estimate the time required to reach 90% of the equilibrium concentration in the sink ($t_{90\%} = \ln(10)/k$), i.e., the time to transfer 45% of the mass from the source to the sink. The velocity rate constant k is proportionally related to the diffusive flux, and is directly related to the permeability P (m h^{-1}), the conductivity g (m h^{-1}) and the transfer coefficient for diffusive transport D in fugacity models (mol h^{-1} Pa^{-1}) (*5*).

Framework for Interpretation of Results. *Diffusion in Water.* The diffusion from the source disk to the sink disk through a layer of water can be described with Fick's first law of diffusion:

$$\frac{dm}{dt} = -A_W \times \frac{D_W}{\Delta x} \times (C_{W1} - C_{W2}) \quad (2)$$

where A_W is the surface area of the water film (m^2), D_W is the diffusion coefficient of the chemical in water (m^2 h^{-1}), Δx is diffusion length (m) and is the thickness of the layer between the disks, and C_{W1} and C_{W2} are the concentrations in the water layer at the upper (1) and lower (2) interface to the PDMS-disk. The following assumptions were made: The water is in local equilibrium with the PDMS-disks at point 1 (source) and point 2 (sink). The concentration ratio between disk and water in equilibrium is described by the partition coefficient K_{DW} (L L^{-1}), where D and W are the indices for the PDMS-disks and water:

$$K_{DW} = \frac{C_D}{C_W} \quad (3)$$

Equations 2 and 3 are combined to

$$\frac{dm}{dt} = -A_W \times \frac{D_W}{\Delta x} \times \frac{1}{K_{DW}} (C_{D1} - C_{D2}) \quad (4)$$

where C_{D1} and C_{D2} are the concentrations in the PDMS-disks at points 1 and 2.

Diffusion in Plant Tissue. With plant tissue as medium between the disks, the transport equation is

$$\frac{dm}{dt} = -A_P \times \frac{D_P}{\Delta x} \times (C_{P1} - C_{P2}) \quad (5)$$

where A_P is the surface area of the plant slice (m^2), D_P is the effective diffusion coefficient of the chemical in plant tissue (m^2 h^{-1}), and C_{P1} and C_{P2} are the concentrations in the plant slice at the upper (1) and lower (2) interface to the PDMS-disk. In phase equilibrium,

$$C_{P1} = C_{D1} \times K_{PD} = C_{D1} \times \frac{K_{PW}}{K_{DW}} \quad (6a)$$

$$C_{P2} = C_{D2} \times K_{PD} = C_{D2} \times \frac{K_{PW}}{K_{DW}} \quad (6b)$$

where K_{PD} is the partition coefficient between plant tissue and disk (kg kg^{-1}), K_{PW} between plant tissue and water (L kg^{-1}), and K_{DW} between disk and water (L L^{-1}). Under the assumption that diffusion only takes place in the water-filled pores (this implies that transport in solids and in air filled pores is negligible, which is the case due to small air pore space and the low K_{AW} of the test chemicals; see the Supporting Information), the effective diffusion coefficient in the plant tissue, D_P, is

$$D_P = D_W \times T_W \times f_W \quad (7)$$

where T_W is a tortuosity coefficient to account for the porosity of the medium, and f_W (kg L^{-1}) is the fraction of chemical dissolved in the water phase of plant tissue, calculated as (*8*)

$$f_W = \frac{C_{W,P}}{C_P} = \frac{W}{K_{PW}} \quad (8)$$

where $C_{W,P}$ is the concentration of the chemical in the water phase of the plant tissue, and W is the pore water fraction of the plant tissue (L kg^{-1}). The tortuosity factor is calculated using the method of Millington and Quirk (cited in ref *9*):

$$T = \frac{W^{10/3}}{(W+G)^2} = W^{4/3} \quad (9)$$

where G is the gas pore volume fraction (L kg^{-1}), which is neglected here. It should be noted that this expression is not unit-true (it probably originates from a regression), which is

ignored here. Summarized,

$$D_P = \frac{D_W \times W^{7/3}}{K_{PW}} \quad (10)$$

We can thus rewrite for the diffusive mass transfer through the plant slice

$$\frac{dm}{dt} = -A_P \times \frac{D_W}{\Delta x} \times \frac{W^{7/3}}{K_{PW}} (C_{D1} - C_{D2}) \times K_{PD} \quad (11)$$

where A_P is the surface area of the plant tissue between the disk (m^2). With $K_{PD} = K_{PW}/K_{DW}$, the partition coefficient plant to water, K_{PW}, can be deleted from the mass balance equation:

$$\frac{dm}{dt} = -A_P \times \frac{D_W}{\Delta x} \times \frac{W^{7/3}}{K_{DW}} (C_{D1} - C_{D2}) \quad (12)$$

Transfer Through Plant Slices versus Transfer Through Water. Directly measurable in the system is the velocity rate constant k (h^{-1}). To obtain the ratio of k-values, and thus the ratio of mass transfer across the plant slice and the water drop, eq 12 can be divided by eq 4:

$$\frac{k_{Plant}}{k_{Water}} = \frac{A_P}{A_W} \times W^{7/3} \quad (13)$$

This means that the mass transfer across the plant tissue in relation to the mass transfer through pure water depends solely on the water content of the plant tissue and the surface area. The partition coefficients are deleted from the equations and do not play any role. This result may be counter-intuitive, but can be tested against the experimental results. A second way to derive this equation is shown in the Supporting Information.

Results and Discussion

Experimental Results. Figure 1 shows the experimentally determined mass transfer from source disk to sink disk. The transfer was fastest for naphthalene, slower and similar for anthracene and phenanthrene, and slowest for fluoranthene. The transfer was faster through carrot than through potato. Rate constants, k, determined for water, potato, and carrot, as medium between the disks are shown in Table 1.

Comparison of Model and Experimental Results. *Diffusion Through Plant Tissue Compared to Diffusion Through Water*. The only input data required to predict the ratio of diffusion through plant tissue to diffusion through water is the plant pore water fraction W. Several data sources were found reporting water contents between 0.778 and 0.833 g/g for potatoes and between 0.882 and 0.95 for carrots (*10*−*12*), indicating differences with variety, origin, and age of the product. Data from the German source (*11*) were used in calculations ($W_{Potato} = 0.778$ and $W_{Carrot} = 0.882$). For carrots, results were also calculated using the Italian source (*12*) because this source reported the highest water content (0.95). No corrections were made for the density of plant material. However, the measured k-values needed to be corrected (by a factor of 2.25) for the difference in surface area between water film (4 mm diameter) and plant slices (6 mm diameter) in the experimental setup.

Tables 2 and 3 show the ratio of measured and predicted k-values for potato to water and carrot to water. For potato (Table 2), the measured ratios (corrected for area) range from 0.43 to 0.64, with a mean of 0.52. With a water content of 0.778, the predicted ratio ($=W^{7/3}$) is 0.56, which is close to the mean of the measured ratios. For carrots (Table 3), the measured ratios vary from 0.79 to 0.96, with a mean of 0.86. The predicted ratio is 0.75 ($W = 0.882$) or 0.89 ($W = 0.95$).

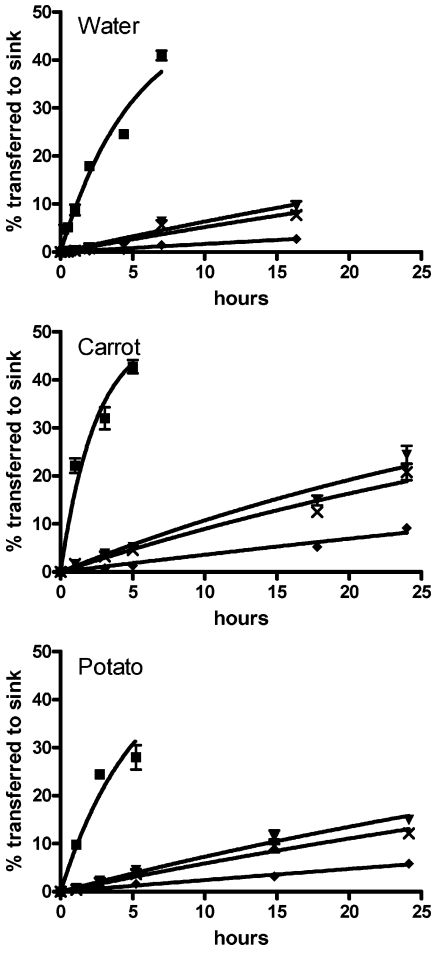

FIGURE 1. Experimentally determined mass transfer for naphthalene (■), phenanthrene (▼), anthracene (×), and fluoranthene (◆) through water, carrot, and potato. Error bars indicate standard error of the mean ($n = 3$). Lines indicate fit curves, from which k-values were derived.

There is no statistically significant difference to the measured ratios (t test, $\alpha = 0.05$).

The rate k can also be calculated using log K_{OW} and M (molar mass) and the properties of the experimental system (ref *5* or Supporting Information). The mean difference between measured and calculated k is 14% only (Supporting Information).

Ratio of Diffusion for Different Chemicals. It was shown that (*5*)

$$k \sim D/K_{DM} \quad (14)$$

where K_{DM} is the partition coefficient between the disk and the matrix. It follows that the ratio of k-values for different chemicals is constant, independent of whether the medium is water, potato, or carrot, and it is

$$\frac{k_A}{k_B} = \frac{D_{WA}/K_{DWA}}{D_{WB}/K_{DWB}} \quad (15)$$

where A and B denote two different chemicals, D_W is the diffusion coefficient in water, and K_{DW} is the partition coefficient between disk and water. The relation between K_{DW} and log K_{OW} is (*7*)

$$\log K_{DW} = \log K_{OW} - 0.91 \quad (16)$$

Subsequently, there should be a linear correlation between log K_{OW} and log k, and the slope should be near −1.0 (the

TABLE 1. Velocity Constants *k* (±Standard Error) Derived for Water, Potato, and Carrot as Medium (h^{-1})

compound	water	potato	carrot
naphthalene	0.199 ± 0.010	0.191 ± 0.017	0.405 ± 0.036
phenanthrene	0.0136 ± 0.0008	0.0158 ± 0.0007	0.0242 ± 0.0013
anthracene	0.0101 ± 0.0008	0.0125 ± 0.0006	0.0198 ± 0.0011
fluoranthene	0.00346 ± 0.00015	0.00499 ± 0.00017	0.00746 ± 0.00042

TABLE 2. Ratios of Measured *k* in Potato to Measured *k* in Water Compared to Predicted Ratios

compound	measured ratio k_P/k_W	corrected for area differences[a]	calculated ratio[b]
naphthalene	0.96	0.43	0.56
phenanthrene	1.16	0.52	0.56
anthracene	1.14	0.51	0.56
fluoranthene	1.44	0.64	0.56
average	1.175	0.52	0.56

[a] Equation 13, $A_p/A_w = 2.25$. [b] Equation 13, ratio = $W^{7/3}$, with water content W is 0.778 (*11*).

TABLE 3. Ratios of Measured *k* in Carrot to Measured *k* in Water Compared to Predicted Ratios

compound	measured ratio k_P/k_W	corrected for area differences[a]	calculated ratio[b]
naphthalene	2.04	0.90	0.75−0.89
phenanthrene	1.78	0.79	0.75−0.89
anthracene	1.80	0.80	0.75−0.89
fluoranthene	2.16	0.96	0.75−0.89
average	1.945	0.86	0.75−0.89

[a] Equation 13, $A_p/A_w = 2.25$. [b]Equation 13, ratio = $W^{7/3}$, with water content W is 0.882 (*11*) to 0.95 (*12*).

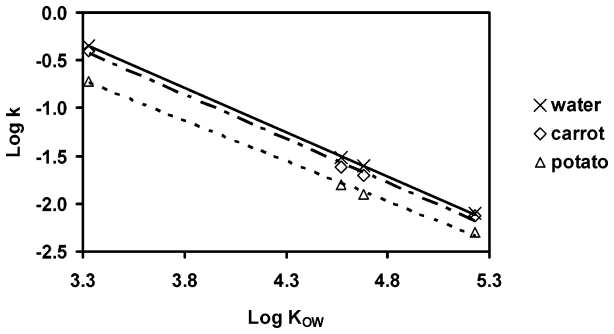

FIGURE 2. Plot of log *k* versus log K_{OW} for the test-chemicals; with trendlines; rate in water corrected for area differences.

slope may deviate slightly from −1 because D in eq 15 depends on the molecule size).

Figure 2 shows the logarithm of the k-values in Table 1, water corrected for difference in area, versus the log K_{OW} of the test chemicals (log K_{OW} data from ref *13*), together with linear trendlines. The regressions yielded are as expected,

$$\text{Water: } \log k = -0.93 \log K_{OW} + 2.74;\ R^2 = 0.999 \quad (17a)$$

$$\text{Potato: } \log k = -0.84 \log K_{OW} + 2.07;\ R^2 = 0.998 \quad (17b)$$

$$\text{Carrot: } \log k = -0.93 \log K_{OW} + 2.67;\ R^2 = 0.996 \quad (17c)$$

there is a highly significant ($p < 0.01$) linear correlation between log k-values and log K_{OW}. This confirms the dominant influence of hydrophobicity on the permeability of PAH in porous media with high water content. The slopes are similar and close to −1 for all media, which confirms the initial assumption that the diffusive mass transfer takes place through the aqueous phase of the tissue. This underlines the validity of both the experimental and the theoretical approach.

Calculation of Diffusion Coefficients Through Plant Tissue. Unknown diffusion constants can be calculated for plant tissue from water content and diffusion coefficient in water. Diffusion coefficients in water can be estimated from the diffusion coefficients of reference compounds (*14*). The water contents of most crops are readily available. Therefore, diffusion coefficients in plant tissue can be derived with ease. Potatoes have gas channels to provide the inner tuber with oxygen (*15*). Thus, the gas phase may be relevant for compounds with higher values of K_{AW} ($>10^{-4}$). However, with our method, the experimental determination of transport in gas channels might prove difficult as gas channels can fill with solution upon cutting slices of potato tissue (L.C. Davis, personal communication).

Difference to Recent Findings. In a similar study (*5*), it was found that humic acids and other dissolved complexing agents enhance the permeability of fluoranthene through an aqueous boundary layer by more than 1 order of magnitude. The increased permeability was due to co-transportation of fluoranthene sorbed or otherwise complexed to such mobile agents. In this study, the aqueous boundary layer was replaced by an immobile plant tissue that instead reduced the permeability.

A Model for Accumulation of Neutral, Lipophilic Compounds in Potatoes. The diffusion coefficients in potatoes can be used to estimate the accumulation of pollutants in this foodstuff. We consider the potato to be a sphere and assume a purely diffusive uptake from soil through the peel.

Generally, the uptake of chemicals from a surrounding medium into an organism can be described by a compartment system:

$$\frac{dC_2}{dt} = k_1 C_1 - k_2 C_2 \quad (18)$$

where k_1 is an uptake rate and k_2 is a depuration rate. In our case, compartment 1 is the soil and compartment 2 is the potato. In steady-state ($dC/dt = 0$), this leads to the equation for the bioconcentration factor BCF

$$\text{BCF} = \frac{C_2}{C_1} = \frac{k_1}{k_2} \quad (19)$$

This BCF describes the situation when forward- and back-diffusion are balanced; the situation is equivalent to phase equilibrium.

Potato is composed of water, carbohydrates, and traces of lipids. The phase equilibrium to water (the partition coefficient potato to water), K_{PW} (L kg^{-1}), can alternatively be estimated from

$$K_{PW} = \frac{C_P}{C_W} = W + f_{CH} \times K_{CH} + L \times a \times K_{OW}{}^{b} \quad (20)$$

where C_P (mg kg^{-1} fresh weight) and C_W (mg L^{-1}) are the chemical concentrations in potato and water; W is the water content of potato (L kg^{-1}); f_{CH} is the fraction of carbohydrates;

L is the lipid content (including waxes and lignin) (kg kg^{-1}); b is an empirical value describing differences between root lipids and n-octanol and is 0.77 (*16*), $a = 1/\rho_{Octanol} = 1.22$ L kg^{-1}; K_{CH} is the partition coefficient of carbohydrates to water. Chiou et al. (*17*) give values for $K_{CH} = 0.1$ for log $K_{OW} < 0$ to $K_{CH} = 3$ for log $K_{OW} > 3$. The carbohydrate fraction usually plays a minor role.

Equation 20 requires as input C_W (mg L^{-1}), the concentration in the water phase of the soil (which is identical to C_{free} in ref *18*). It can be estimated from the concentration in bulk soil, C_S (mg kg^{-1}), using the partition coefficient K_{SW} (L kg^{-1}):

$$K_{SW} = \frac{C_S}{C_W} = \frac{f_{OC} \times K_{OC} \times \rho_{dry} + W_S}{\rho_{wet}} \quad (21)$$

Where f_{OC} is the fraction of organic carbon (kg kg^{-1}); ρ is the density of the soil (wet or dry, kg L^{-1}); W_S is the volume fraction of water in the soil (L L^{-1}); K_{OC} (L kg^{-1}) is the partition coefficient between organic carbon and water and can be estimated from ref *19*

$$\log K_{OC} = 0.81 \times \log K_{OW} + 0.1 \quad (22)$$

The equilibrium BCF of potatoes (kg kg^{-1}) in soil can then be calculated from the ratio of eqs 20 and 21:

$$BCF = \frac{C_P}{C_S} = \frac{K_{PW}}{K_{SW}} \quad (23)$$

From the radial diffusion model, an estimate for k_2 can be deduced (*20*)

$$k_2 = \frac{23 \times D_2}{R^2} \quad (24)$$

where D_2 is the diffusion coefficient of the chemical in compartment 2, here D_P (eq 10); R is the radius of the potato (m). Now follows for k_1 from eq 19:

$$k_1 = k_2 \times BCF \quad (25)$$

Equations 19 or 23 describe the equilibrium between uptake and depuration of a compound, which is here identical to the equilibrium between potato and soil. Additional processes, i.e., first order degradation, may be added. For potatoes, dilution by growth is relevant. For exponential growth, the growth rate k_G can be added to the depuration rate, and the steady-state concentration ratio (bioaccumulation with growth) BCF*, is

$$BCF^* = \frac{k_1}{k_2 + k_G} \quad (26)$$

Figure 3 shows a calculation of the BCF and BCF* potato to soil versus log K_{OW} using the data given in Table 4. For very polar compounds, the calculated *BCF* is > 1, due to the higher water content of potatoes, compared to soil. For more lipophilic compounds, the BCF decreases. This is due to the low lipid content of potatoes (0.1%), relative to the f_{OC} of soil (2.3%). For log $K_{OW} > 4$ there is an increasing difference between BCF (equilibrium) and BCF* (with growth). This is because the depuration rate k_2 (calculated from the diffusion coefficient in potatoes) decreases with increasing log K_{OW} (increasing K_{PW}), while the growth rate is independent of chemical properties. A reduced accumulation of lipophilic compounds due to growth was seen before for carrots (*21*) and algae (*22*) and may provide a plausible explanation for the partition-limitation of the uptake of organic chemicals into crops described by ref *17*.

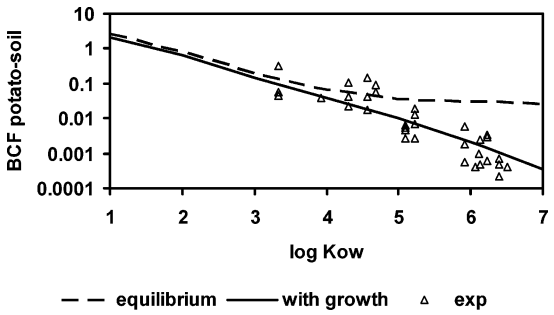

FIGURE 3. Calculated BCF potato-soil with and without (equilibrium) growth versus log K_{OW}; exp are experimental results for potato cores (*23*).

TABLE 4. Data for BCF Calculation

parameter	symbol	value	unit	reference
potato water content	W	0.778	L kg^{-1}	*11*
potato lipid content	L	0.001	kg kg^{-1}	*11*
potato fraction of carbohydrates	f_{CH}	0.154	kg kg^{-1}	*11*
potato growth rate	k_{Growth}	0.139	d^{-1}	arbitrary[a]
potato radius	R	0.04	m	arbitrary
soil organic carbon content	f_{OC}	0.023	kg kg^{-1}	*23*[b]
soil pore water	W_S	0.35	L L^{-1}	arbitrary
soil wet density	ρ_{wet}	1.95	kg L^{-1}	arbitrary
soil dry density	ρ_{dry}	1.6	kg L^{-1}	arbitrary
molar mass	M	200	g mol^{-1}	average for PAH

[a] Calculated from a potato doubling time of 5 days. [b] Calculated from organic matter OM 3−5% using the relation f_{OC} = OM/1.724

Figure 3 shows also BCF-values determined in field experiments (*23*). Four potato varieties had been obtained from organic farms in England. Care was taken to collect soil immediately surrounding the potatoes. Potatoes were peeled with a vegetable peeler to a depth of 2 mm before analysis. Plotted is the ratio of concentrations in potato cores to soil for 13 PAHs (naphthalene, acenaphthylene, acen/fluorene, phenanthrene, fluoranthene, pyrene, benzo[*a*]anthracene, benzo[*b*]fluoranthene, benzo[*k*]fluoranthene, benzo[*a*]pyrene, indeno[1,2,3-*c,d*]pyrene, dibenzo[*a,h*]anthracene, and benzo[*g,h,i*]perylene). Results below the limit of detection were omitted. Log K_{OW}-values were taken from (*13*), and if not available there, from ref *24* or *25*. As predicted by the model, the measured BCFs of the PAHs decrease with increasing log K_{OW} from values near 0.1 to below 10^{-3}. At very high log K_{OW}, the model tends to overestimate the BCF. One plausible reason herefore is the 2 mm peeling of the potatoes: the concentrations of the immobile lipophilic PAHs were highest in or near the peel (*23*). Another reason might be that freely dissolved pore water concentrations of field-contaminated soils may be lower than predicted by the K_{OC}-regression (*26*).

Underlying Assumptions and Limitations of the Potato Model. The new model approach requires several assumptions and is, therefore, limited in its applicability. The model is only valid for neutral organic compounds. Translocation of chemicals in the phloem, as it may occur for weak acids and polar neutral compounds, was excluded. The concentration in soil pore-water was calculated from K_{OC}; hereby, reduced bioavailability, for example, due to aging, was not considered. In field-contaminated soils, pore-water concentrations can be much lower and soil sorption coefficients can be much higher than equilibrium partitioning models predict (*26*). Also, a depletion of the soil due to uptake into potato was not taken into consideration. If such processes are of relevance, they should be included in the calculation of soil pore-water concentrations. Metabolism of the chemical

inside the potato was not taken into account, but can be added as a process. The model is based on a steady-state solution and, therefore, cannot consider differences in time and space, such as differences between outer and inner potato tissue. If concentrations depending on space and time are required, the solution in the Supporting Information might be used. Summarized, the potato model in its present formulation should only be applied to persistent neutral organic chemicals.

A new method for quantifying the effect of medium composition on the diffusive mass transfer of hydrophobic organic chemicals through thin layers was applied to plant tissue. The results were reproducible with small standard errors. Diffusion through potato was slower than diffusion through carrot. The diffusion velocity in relation to water could be quantified and predicted with tissue water content as the sole descriptor. The resulting diffusion coefficients were used to estimate the accumulation of PAH in potatoes. For lipophilic compounds, the BCF was reduced due to transport limitation and growth. This is in agreement with field results for PAHs.

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Supporting Information Available

A figure of the experimental system, methods to calculate the rate k and the diffusion in gas phase, an alternative method to derive eq 14, and an earlier version of the potato model, which treats the problem of diffusion into a sphere dependent on space and time. This material is available free of charge via the Internet at http://pubs.acs.org.

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