Appendix 4F
Plant uptake

1.1 Overview

The uptake of contaminants by plants is a complex biological process. There is no accurate, theoretically robust model for predicting the concentration of a contaminant in plant material, however, empirical formula have been derived by numerous sources to simulate contaminant uptake by plants.

A number of models are available for the uptake of contaminants by plants (e.g. HESP (Shell, 1994), CAPCOA (1992)), but in general they reduce to empirical correlations (e.g. Travis (1988), Ryan et al (1988)) and hence are limited by the relevance of the source data on which they are based.

For the purposes of this appendix the following approach has been adopted:

- modelling the distribution of contaminants between the soil moisture, adsorbed and vapour phases in soil using a fugacity approach (HESP (1994))
- modelling the uptake of contaminants by plants using the relationship developed by Ryan et al (1988)
- comparison with published contaminant concentrations in soil and plants.

The Ryan et al (1988) model was selected on the basis that it relates plant uptake to pore water concentrations, and therefore, when combined with a partitioning relationship can account for differences in soil type. In contrast the Travis (1988) model depends on Kow only. In addition, Ryan considers a range of chlorinated and non-chlorinated compounds in derivation of the correlation, whereas the Travis relationship is based largely on chlorinated compounds.

Patterson (1989) developed a similar approach based on fugacity partitioning and use of an empirical correlation, however modifications to the empirical correlation incorporated in the Patterson model result in prediction of high level of uptake for highly lipophilic compounds such as benzo(a)pyrene. Further benzo(a)pyrene lies outside the Kow range for the chemicals used in deriving the empirical correlation use.

As discussed in Module 4, the uptake of contaminants by plants has only been considered for the PAH compounds i.e. naphthalene, pyrene and benzo(a)pyrene. The BTEX compounds are not expected to persist in surface soils used for gardening (i.e. regularly watered, fertilised and aerated).

For the purposes of this module only contamination of a uniform surface soil is considered, representing a range of garden soils. In particular the organic carbon content of the soil has been increased to allow for the use of compost and other organic supplements in gardens.

1.2 Phase partitioning in the soil environment

HESP (1994) uses a fugacity approach to phase partitioning based on the Mackay level 3 fugacity model. The fugacity and phase compositions are calculated as follows:

$$Z_a = \frac{1}{R \times T_{soil}} \quad \text{[F1]}$$

$$Z_w = \frac{S(T)}{P(T)} \quad \text{[F2]}$$

where

$P(T)$ = vapour pressure at T_{soil} (Pa)

$S_w(T)$ = solubility in water at T_{soil} (mg/L)

$S(T)$ = $S_w(T)/M$ (mole/m^3)

Z_a = fugacity capacity constant air (mole/m^3.Pa)

Z_w = fugacity capacity constant water (mole/m^3.Pa)

R = gas constant (8.3143) (Pa.m^3/mole.K)

T_{soil} = temperature of the soil (°K) -assumed 298 °K

or $$Z_w = \frac{1}{H_s} \quad \text{[F3]}$$

where H_s = Henry's constant corrected for temperature. In this application it is assumed that the soil temperature is the same as the reference temperature (298K) and so no correction is necessary.

$$Z_s = \frac{K_{oc} \times f_{oc} \times SG \times Z_w}{SN_s} \quad \text{[F4]}$$

where

Z_s = fugacity capacity constant soil (mole/m^3.Pa)

K_{oc} = partition coefficient for octanol-water (dm^3/kg)

f_{oc} = fraction organic carbon

SG = specific gravity (g/cm^3)

SN_s = volume phase of solid phase

$$P_a = \frac{Z_a \times SN_a}{Z_a \times SN_a + Z_w \times SN_w + Z_s \times SN_s} \quad \text{[F5]}$$

$$P_w = \frac{Z_w \times SN_w}{Z_a \times SN_a + Z_w \times SN_w + Z_s \times SN_s} \quad \text{[F6]}$$

$$P_s = \frac{Z_s \times SN_s}{Z_a \times SN_a + Z_w \times SN_w + Z_s \times SN_s} \quad \text{[F7]}$$

where

P_a = mass fraction in soil gas phase

P_w = mass fraction in soil liquid phase (water)

P_s = mass fraction in soil solid phase

SN_a = volume phase of gas fraction

SN_w = volume phase of liquid phase

SN_s = volume phase of solid phase

$= 1 - SN_a - SN_w$

The soil type used for the model calculations is standard soil 10% OM, used by the Netherlands (HESP). This is expected to be reasonably typical of garden soils amended with organic supplements (e.g. compost). A list of the soil parameters used are presented in Table 4F3.

Table 4F1 **Plant uptake soil parameters**

Parameter	Standard Soil 10% OM
SG - kg/dm^3	1.5
SNa	0.2
SNw	0.2
foc	0.058

1.3 Uptake model

The reference to Ryan et al, 1988 is used for modelling the uptake of contaminants by plants.

Ryan et al produced correlations between the contaminant concentration in the soil water and that in produce based on published information on the uptake of chemicals by plants. The chemicals used during the tests were mainly pesticides, of lower octanol-water values than the chemicals considered in this model, however, in some cases the chemicals included extend to species more similar to the chemicals of interest than in the case for other models. The Ryan model has been found to produce predictions of uptake closer to published data (Edwards (1983)) than other references.

Ryan et al. define a root concentration factor:

$$\text{RCF} = \frac{\text{concentration in root } (\mu\text{g / g fresh wt})}{\text{concentration in external solution } (\mu\text{g / mL})} \qquad \text{[F8]}$$

The RCF is estimated by the following correlation:

$$\log(\text{RCF} - 0.82) = 0.77 \log K_{ow} - 1.52 \qquad \text{[F9]}$$

where K_{ow} = octanol-water partition coefficient

Likewise, a stem concentration factor is defined as:

$$\text{SCF} = \frac{\text{concentration in stem } (\mu\text{g / g fresh wt})}{\text{concentration in external solution } (\mu\text{g / mL})} \qquad \text{[F10]}$$

The SCF is estimated using the following correlation:

$$\left[10^{(0.95 \log Kow - 2.05)} + 0.82\right] \times (0.784) 10^{\frac{-0.434(\log Kow - 1.78)^2}{2.44}} \qquad \text{[F11]}$$

The calculated RCF and SCF are combined to give a weighted plant uptake factor (PUF). The weightings are based on the range of home-grown produced food types in Australia (ABS, 1994). Weighting is given as follows:

- root crops are subject to root uptake characterised by the RCF
- close to ground fruits and vegetables (e.g. strawberries, radishes), and vines (e.g. tomatoes, beans) are subject to uptake and translocation described by the SCF
- tree fruits (e.g. apples, lemons) are not subjected to uptake (deposition not considered).

The proportions of home-grown produce in Australia were calculated from the Australian Bureau of Statistics (ABS) and are presented in Table 4F2.

Table 4F2 Home-grown produce types

Food Type	Proportion Percent
root crops	10
other fruit and vegetables	50
tree fruits	40

The PUF is calculated using the following relationship:

$$PUF = f_r \times RCF + f_s \times SCF \qquad [F12]$$

where f_x = fraction produce type x

and plant concentration is calculated by:

$$C_p = PUF \times C_t \qquad [F13]$$

where C_t = total measured soil concentration

1.4 Review of published information

The uptake of contaminants by plants is plant species, chemical and site specific and hence there is considerable variability in the published uptake information. The following information is drawn from a review article by Edwards (1983) unless otherwise specified:

- The published ratios of benzo(a)pyrene concentrations in plants to that in soil range from 0.002 to 0.33, corresponding to concentrations in the plant material of 0.1 to 150 µg/kg (fresh basis, typically 1 to 10 µg/kg).
- The published ratios of total PAH concentrations in plants to that in soil range from 0.001 to 0.183 (fresh basis).
- Travis and Arms (1988) used a ratio of plant concentration to soil concentration 0.05 as part of the development of an empirical correlation.
- Actively growing green plant parts may naturally contain in the range 10 to 20 µg/kg benzo(a)pyrene, but storage tissues generally contain 1-10% of that in green plant portions
- Washing typically removes less than 25% of the PAHs from vegetables.
- PAH concentrations in plant skin and peel are higher than those in internal tissues.
- Most PAH contamination of vegetation occurs through atmospheric deposition.

For comparison the benzo(a)pyrene concentrations corresponding to an incremental lifetime risk of cancer of one in 100,000 are in the range 0.5 to 5 μg/kg fresh basis (refer Appendix 4G).

The predicted uptake of contaminants using the Ryan model as outlined above is broadly consistent with the published total benzo(a)pyrene concentrations, but the published information accounts for naturally occurring benzo(a)pyrene and the contribution from other sources (e.g. atmospheric deposition). On this basis the Ryan model may be regarded reasonable, although depending on the significance of other sources it may be conservative. It is of note that the benzo(a)pyrene concentrations in produce corresponding to an incremental lifetime risk of cancer of one in 100,000 for the exposure scenarios considered are of the same order or less than concentrations that may be naturally occurring.

1.5 References

Australian Bureau of Statistics. 1994**. Home Production of Selected Foodstuffs, Australia, Year Ended April 1992**, Catalogue No 7110.0

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Patterson S., and Mackay, D. 1989. **Modelling the uptake and distribution of organic chemicals in Plants**, In Allen, D.T. et **al Intermedia Pollutant Transport: Modelling and Field Measurements**, Plenum Press, New York, pp 269 - 282.

Ryan, J.A., Bell, R.M., Davidson, J.M., & O'Connor, G.A. 1988. **Plant uptake of non-ionic organic chemicals from soils**, Chemosphere Vol 17, 2299 - 2323.

Shell. 1994. **The concepts of HESP, Reference Manual, Human Exposure to Soil Pollutants, Version 2.10a.**

Toxics Committee of the California Air Pollutant Control Officers Association. 1993. **CAPCOA, Air Toxics "Hot Spots" Program, Revised 1992 Risk Assessment Guidelines.**

Travis C.C., and Arms A.D. 1988. **Bioconcentration of Organics in Beef, Milk and Vegetation**, Environ. Sci. Technol., Vol. 22 No. 3, 271-274.

Table 4F3 Plant uptake of PAHs

Soil Parameters	
SG (t/m^3)	1.5
Sna	0.2
SNw	0.2
Foc	0.058

Chemical Parameters	Naphthalene	Pyrene	Benzo(a)pyrene
Koc	8.44E+02	2.50E+04	1.31E+05
log(Kow)	3.37	5.18	6.04
S (mg/L)	31	0.132	0.0038
P (atm)	3.63E-04	1.17E-07	2.10E-10
MW (g/mol)	12819	202.3	252.3

Consumer Parameters	
fraction root	0.1
fraction stem	0.5
fraction leaves/fruit	0.4

Fugacity Calculations	H (Pa.m^3/mol)	Za	Zw	Zs	Pa	Pw	Ps
naphthalene	15210	4.04E-04	6.57E-05	8.05E-03	1.64E-02	2.67E-03	9.81E-01
pyrene	18.17	4.04E-04	5.50E-02	2.00E+02	6.74E-07	9.19E-05	1.00E+00
benzo(a)pyrene	1.413	4.04E-04	7.08E-01	1.34E+04	1.00E-08	1.75E-05	1.00E+00

Plant Concentration Calculations	BCFroot	BCFstem	BCFave
naphthalene	2.55E-01	8.36E-02	6.73E-02
pyrene	2.03E-01	3.53E-03	2.21E-02
benzo(a)pyrene	1.78E-01	2.98E-04	1.79E-02