PCB TRANSFER FROM AIR TO GRASS: FIELD EVALUATION OF TWO MATHEMATICAL MODELLING APPROACHES

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INTRODUCTION

The air-to-grass-to-cattle food chain constitutes an important pathway of human exposure to SOCs like PCBs. This paper evaluates the ability of two mathematical modelling approaches previously applied to PCDD/Fs, to predict the relationship between levels of 20 individual PCBs in a temporally and spatially consistent dataset comprising air and grass samples taken over a 4 month period at an urban site in Birmingham, UK.

EXPERIMENTAL METHODS

Sampling protocols

Samples of air, bulk (*i.e.* wet and dry) atmospheric deposition, and grass were taken from the same urban location *ca* 3 km from the centre of Birmingham. A total of 12, 4 and 4 samples of air, bulk atmospheric deposition, and grass respectively were collected between 24th June and 10th November 1997. The mean air temperature over the full duration of the experiment was 286.6K, the mean dry weight fraction of grass was 0.19, and the mean fresh weight grass yield was 185 g m^{-2}. Each air sample was taken over a separate 24 h period at regular intervals throughout the experiment using a Graseby-Andersen Hi-Vol sampler modified to hold a Teflon coated glass-fibre filter (GFF, 0.6 μm pore size) and a pre-cleaned polyurethane foam (PUF) plug. Sampling flow-rates were 0.7 - 0.9 m^3 min^{-1} yielding sample volumes of *ca* 1000 - 1300 m^3. The bulk deposition sampling apparatus consisted of a glass vessel connected to an inverted frisbee, whilst grass samples were harvested from a "fenced-off" 1 m^2 plot.

Sample Purification and Analysis

PCB analyses were conducted using well-validated containment-enrichment, GC/MS procedures reported elsewhere[1]. Bulk deposition samples were filtered using a glass fibre filter in series with a PUF plug. The two phases were analysed separately to provide measurements of dissolved and particle phase deposition fluxes.

RESULTS & DISCUSSION

The mean concentrations of selected PCB congeners measured in air (sum of vapour and particulate-bound phases), operationally-defined atmospheric particle-bound deposition (D_p), and grass over the entire sampling event are given in Table 1. Also included are levels in grass predicted using the air-to-grass component of an empirical air-to-foodstuff mathematical model originally developed for PCDD/Fs[2], and adapted for use with PCBs. Space restrictions preclude a detailed account of the model structure and algorithms, but in summary, it uses bulk (*i.e.* sum of vapour and particulate phases) air concentrations as its principal source term. Algorithms based on those of Junge[3] are used to predict atmospheric phase distribution, using temperature-corrected P_l values calculated according to Falconer and Bidleman[4]; an air-to-leaf transfer factor (B_{vpa}) is calculated based on algorithms reported by Lorber *et al*[5] and published values of K_{ow} and H[6,7,8]; particle-bound (dry and wet) atmospheric deposition is calculated using previously published washout coefficients and deposition velocities[9,10], and used to predict plant uptake from particulates deposited on foliage; and finally, root uptake and subsequent translocation is forecast using soil concentrations (those used are those reported for the same site in reference 1) as source term, alongside a K_{ow}-based root concentration factor.

Clearly, there is good agreement (*i.e.* observed:predicted ratios = 0.34 - 1.97; mean = 0.93; $\sigma = 0.46$) between observed grass concentrations and those predicted by the model. Similar correlation between model predictions and measured values exist for other key parameters: *viz* fraction of airborne concentration that is particle-bound (observed:predicted ratios = 0.17 - 2.15; mean = 0.89; $\sigma = 0.59$), and particle deposition fluxes (observed:predicted ratios = 0.33 - 4.19; mean = 1.33; $\sigma = 1.09$).

Other authors have suggested that air-to-grass transfer of PCDD/Fs may be predicted by means of a simple scavenging approach[11,12]. To evaluate the applicability of a similar approach to PCBs, we plotted observed PCB levels in air versus those in grass for: (a) tri- and tetrachlorobiphenyls; and (b) penta- and hexachlorobiphenyls - Figures 1 and 2 respectively. These data demonstrate that the scavenging approach may be successfully applied to penta- and hexachlorobiphenyls (*i.e.* the grass in our experiment scavenged the PeCBs and HxCBs present in 22 m^3 of air), but not tri- and tetrachlorinated congeners.

This paper demonstrates that an empirical equilibrium partitioning modelling approach predicts air-to-grass transfer of PCBs with reasonable accuracy. Interestingly however, although the simple scavenging approach successfully employed for PCDD/Fs by other workers appears inappropriate for predicting air-to-grass transfer of tri- through tetrachlorobiphenyls, it appears to be applicable to penta- and hexachlorobiphenyls. Although the accuracy of the modelling approaches evaluated is encouraging, more work is required if air-to-grass transfer of these important chemicals is to be fully understood.

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REFERENCES

1. Ayris, S, Currado, G, Smith, D and Harrad, S; *Chemosphere*, **1997**, 35, 905.
2. Harrad, S and Smith, D; *Chemosphere*, **1997**, 34, 1723.
3. Junge, C. p. 7-26, in *Fate of pollutants in the air and water environments, Part I*, Ed. I.H. Suffet, Wiley, 1977.
4. Falconer, R.L and Bidleman, T.F; *Atmos. Environ.*, **1994**, 28, 547.
5. Lorber, M, Cleverly, D, Schaum, J, Phillips, L, Schweer, G and Leighton, T; *Sci. Tot. Environ.*, **1994**, 156, 39.
6. Hawker, D. W and Connell, D. W; *Environ. Sci. Technol.*, **1988**, 22, 398.
7. Ballschmiter, K and Wittlinger, R; *Environ. Sci. Technol.*, **1991**, 25, 1103.
8. Shiu, W. Y and Mackay, D; *J. Phys. Chem. Ref. Data*, **1986**, 15, 911.
9. Ligocki, M. P and Pankow J. F; *Environ. Sci. Technol.*, **1989**, 23, 75.
10. Holsen, T. M, Noll, K.E, Liu, S-P and Lee, W-H; *Environ. Sci. Technol.*, **1991**, 25, 1075.
11. McLachlan, M.S; *Organohalogen Compds.*, **1995**, 26, 105.
12. Jones, K.C and Duarte-Davidson, R; *Environ. Sci. Technol.*, **1997**, 31, 2937.

Table 1: Observed PCB Concentrations in Air, D_p, Grass, and Levels in Grass Predicted by Equilibrium Partitioning Model

PCB #	Air (ng m^{-3})	Dp (ng m^{-2} yr^{-1})	Predicted Grass (ng kg dw^{-1})	Observed Grass (ng kg dw^{-1})
33	0.0144	250	97	120
22	0.0073	140	44	82
49	0.0090	160	105	160
44	0.0110	230	102	160
41/64	0.0102	300	149	130
74	0.0047	110	122	82
66	0.0068	220	175	160
95	0.0135	370	286	260
91	0.0017	55	36	34
84/92	0.0021	84	51	42
99/113	0.0055	180	200	120
97	0.0032	170	88	95
87	0.0053	190	143	120
110	0.0145	510	591	360
118	0.0076	310	497	230
105	0.0021	150	98	92
151	0.0019	69	113	46
149	0.0067	220	364	150
153	0.0060	250	468	160
132	0.0021	100	77	51

Figure 1: Relationship between Grass & Air Levels for T3CBs & T4CBs

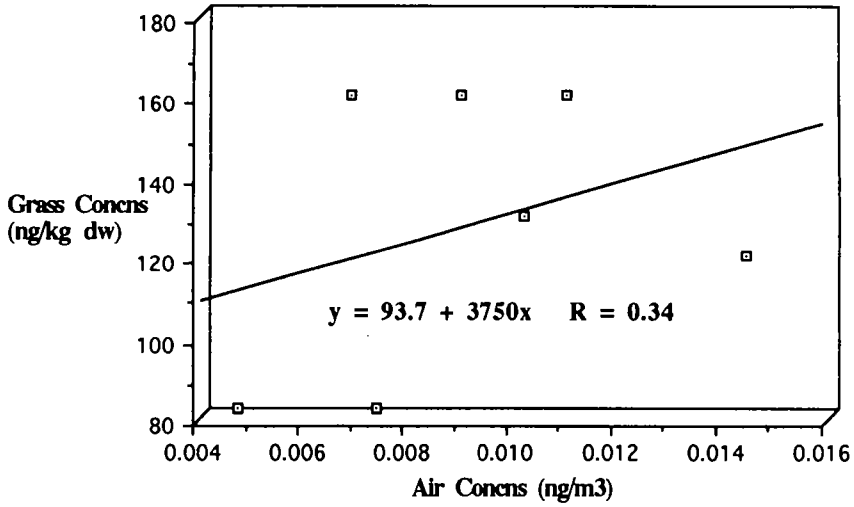

Figure 2: Relationship between Grass & Air Concentrations for PeCBs & HxCBs