# EVALUATION OF A TERRESTRIAL FOOD CHAIN MODEL FOR PCDD/Fs

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## 1. Introduction

This paper evaluates a model designed to predict PCDD/F transfer through the terrestrial food chain, using air and soil concentrations to forecast levels in foodstuffs. The model's validity is assessed by comparison of predicted and observed foodstuff concentrations, and *via* comparison of the model's estimate of total UK human exposure with those based on measured foodstuff concentrations.

## 2. Structure/Assumptions of Model

The basic structure of the model is that used by Lorber *et al* in their air-to-beef food chain model[1)], but extended to incorporate predictions of transfer from air and soil to milk, eggs, poultry, and both above- and below-ground food crops. Although space restrictions preclude detailed description of the individual algorithms and input data used in the model, a glossary of some of the terms used and their definitions is given in Table 1, whilst Figure 1 illustrates the basic model structure. One of the features of the model is the inclusion of homologue-specific values for particle washout coefficients and deposition velocities, which exert a significant influence on the contribution of dry particle deposition to PCDD/F concentrations in grass. The influence of feedlot fattening - whereby animals are fed an essentially residue-free grain diet for a period prior to slaughter - on PCDD/F concentrations in retail meat, is addressed by assuming a first order elimination process.

$$i.e.\ C_t = C_0 * \exp(-kt)$$

**Table 1: Glossary of Selected Terms Used**

| | |
|---|---|
| $C_t$ | concentration at time t |
| t | duration of the feedlot fattening process; assumed here to be 120 d |
| $C_0$ | concentration at t = 0; *i.e.* before feedlot fattening |
| k | congener-specific first order elimination rate constant ($d^{-1}$), derived from data supplied by Olling (personal communication) |
| $C_g$ | total PCDD/F concentration in grass (ng $kg^{-1}$ dry weight (dw)) |
| $C_r$ | contribution to $C_g$ arising from root uptake (ng $kg^{-1}$ dw) |
| $C_p$ | contribution to $C_g$ arising from wet and dry particulate deposition (ng $kg^{-1}$ dw) |
| $C_v$ | contribution to $C_g$ arising from dry gaseous deposition (ng $kg^{-1}$ dw) |
| $C_{rm}$ | PCDD/F concentration in "retail" meat - *i.e.* after feedlot fattening (ng $kg^{-1}$ fresh weight (fw)) |
| $C_{mi}$ | PCDD/F concentration in milk (ng $kg^{-1}$ fw) |
| $C_c$ | PCDD/F concentration in chicken meat (ng $kg^{-1}$ fw) |
| $C_{eb}$ | PCDD/F concentration in chicken eggs (ng $kg^{-1}$ fw) |

## 3. Results

The model assumes that grass concentrations are the sum of contributions resulting from: (a) root uptake from soil; (b) dry gaseous atmospheric deposition, and (c) wet and dry particle atmospheric deposition. Table 2 shows the results of an attempt to evaluate the efficacy of the equations employed to forecast grass concentrations, by comparing predicted and observed grass concentrations, along with listing the relative contribution of the three uptake pathways to total predicted grass concentrations. This latter "check" is important, as recent work by Welsch-Pausch *et al* has demonstrated dry gaseous deposition to be the most significant uptake pathway for PCDD/Fs into Welsh rye grass[2]. In this respect, the predictions of our model are encouraging, as they show only a very minor contribution from root uptake, with the vast majority of PCDD/Fs in grass foliage predicted to arise from dry gaseous deposition. Uptake from particle deposition is predicted to play a minor rôle, which - as indicated by the experimental work of Welsch-Pausch *et al* [2]- increased in importance with increasing chlorination. Furthermore, the model's ability to forecast $C_g$ is considered reasonably satisfactory, with predicted concentrations for all bar three congeners falling within an order of magnitude of the "observed" values used for comparison.

Table 3 shows how model predictions of PCDD/F levels in various foodstuffs compare with "observed" values. Whilst model performance for foodstuffs of animal origin is satisfactory in terms of $\Sigma$i-TE, there is considerable variation in accuracy for individual congeners, thus indicating that there remains considerable scope for model improvement. As a final "check" on model performance, total daily UK human exposure to PCDD/Fs was estimated by multiplying the model's predictions of concentrations in foodstuffs by the estimated typical daily quantity consumed[3]. The model's estimate amounts to 124 pg $\Sigma$i-TE, which compares reasonably closely with the most recent estimate of 69 pg $\Sigma$i-TE derived for a "basket" of foodstuffs - excluding fruit and vegetables - by MAFF[4].

## 4. Conclusions

Whilst models of this type are reasonably accurate in terms of $\Sigma$i-TE, this masks a lack of understanding of the behaviour of PCDD/Fs within the terrestrial food chain. Although the development of "100% accurate" models is beyond our current capabilities, all aspects of transfer between different trophic levels require more detailed study, as transfer factors used are based on a very limited database of experimental data, and little is known about the transfer into livestock animals other than cattle and chickens. Another factor limiting the development of such models is the dearth of data suitable for evaluation purposes - *i.e.* spatially and temporally internally-consistent data sets recording PCDD/F concentrations in air, soil, deposition, grass and foodstuffs - and the conduct of carefully-targeted experimental programmes to provide such information is considered a research priority.

## 5. References

1) Lorber, M., Cleverly, D., Schaum, J., Phillips, L., Schweer, G., and Leighton, T. (1994): Development and validation of an air-to-beef food chain model for dioxin-like compounds, Sci. Tot. Environ. 156, 39-65.

2) Welsch-Pausch, K., McLachlan, M.S., and Umlauf, G. (1995): Determination of the Principal Pathways of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans to Lolium Multiflorum (Welsh Rye Grass), Environ. Sci. Technol. 29, 1090-1098.

3) Ministry of Agriculture, Fisheries and Food (MAFF) (1988): The British Diet: Finding the Facts, Food Surveillance Paper No. 23, pubd. HMSO, London.

4) Ministry of Agriculture, Fisheries and Food (MAFF) (1995): Dioxins in Food: UK Dietary Intakes, Food Surveillance Information Sheet No. 71.

5) Kjeller, L-O., Jones, K.C., Johnston, A.E., and Rappe, C. (1991): Increases in the polychlorinated dibenzo-p-dioxin and -furan content of soils and vegetation since the 1840s, Environ. Sci. Technol, 25, 1619-1626.

6) Ministry of Agriculture, Fisheries and Food (MAFF) (1992): Dioxins in Food, Food Surveillance Paper No. 31, pubd. HMSO, London.

## 6. Acknowledgement

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**Figure 1: Basic Structure of Terrestrial Food Chain Model**

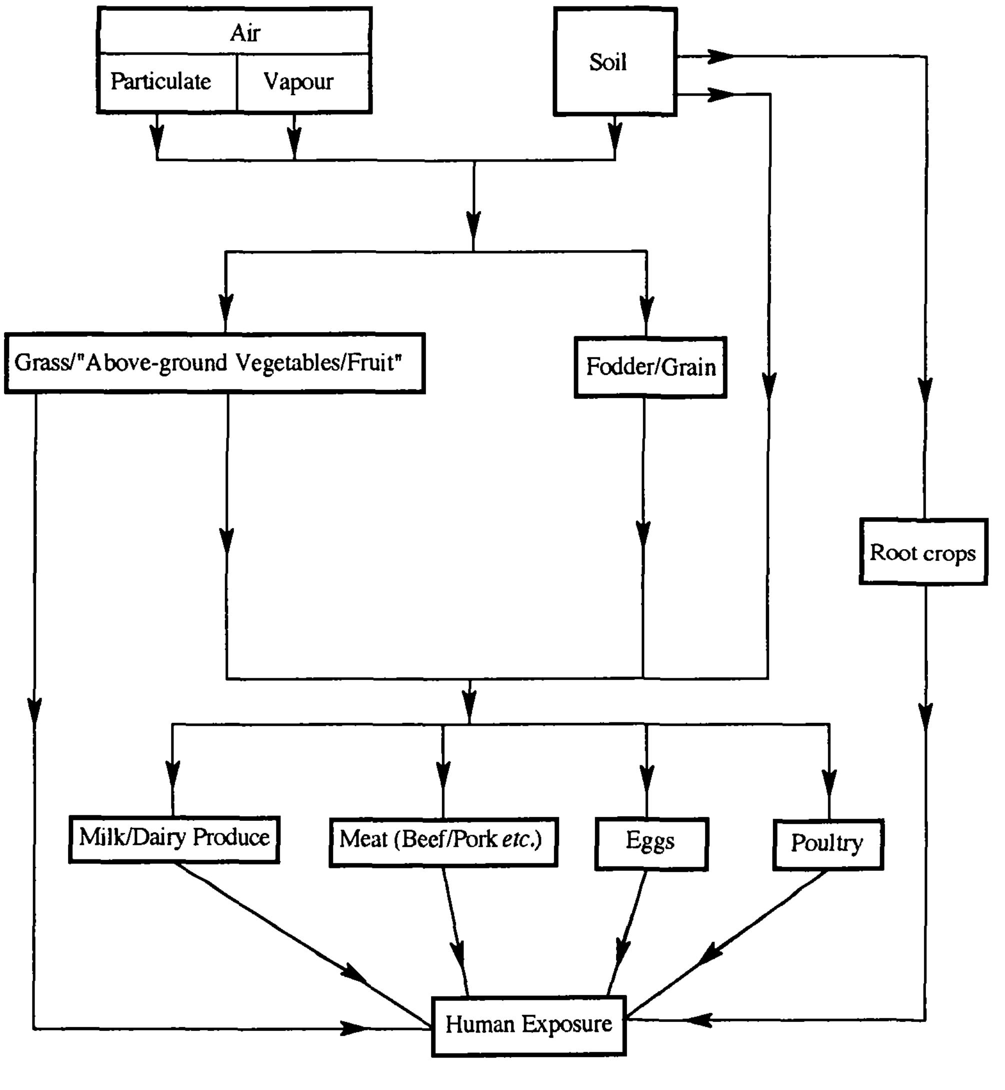

**Table 2: Contribution of Different Uptake Pathways to Predicted Grass Concentrations and Comparison with "Observed" Grass Concentrations**

| | % Contribution to $C_g$ from... | | | | "Observed" Grass |
|---|---|---|---|---|---|
| **Congener** | $C_r$ | $C_p$ | $\dot{C}_v$ | $C_g$ | **Concentration**[a] |
| 2,3,7,8-TCDD | 2.13 | 0.61 | 97.3 | 0.03 | 0.03 |
| 1,2,3,7,8-$P_eCDD$ | 0.44 | 1.54 | 98.0 | 0.38 | 0.14 |
| 1,2,3,4,7,8-$H_xCDD$ | 0.17 | 1.14 | 98.7 | 0.26 | 0.14 |
| 1,2,3,6,7,8-$H_xCDD$ | 0.31 | 2.41 | 97.3 | 0.25 | 3.0 |
| 1,2,3,7,8,9-$H_xCDD$ | 0.53 | 4.50 | 95.0 | 0.21 | 1.4 |
| 1,2,3,4,6,7,8-$H_pCDD$ | 0.39 | 5.80 | 93.8 | 1.5 | 5.9 |
| OCDD | 0.19 | 4.50 | 95.3 | 8.8 | 24 |
| 2,3,7,8-TCDF | 0.11 | 0.23 | 99.7 | 5.8 | 0.46 |
| 1,2,3,7,8-$P_eCDF$ | 0.67 | 0.69 | 98.7 | 0.73 | 0.18[b] |
| 2,3,4,7,8-$P_eCDF$ | 0.72 | 1.15 | 98.1 | 0.50 | 0.20 |
| 1,2,3,4,7,8-$H_xCDF$ | 1.35 | 2.89 | 95.8 | 0.22 | 0.32[c] |
| 1,2,3,7,8,9-$H_xCDF$ | 0.09 | 1.58 | 98.3 | 0.03 | 0.02 |
| 1,2,3,6,7,8-$H_xCDF$ | 1.27 | 2.72 | 96.0 | 0.15 | 0.16 |
| 2,3,4,6,7,8-$H_xCDF$ | 1.59 | 2.63 | 95.8 | 0.11 | 0.15 |
| 1,2,3,4,6,7,8-$H_pCDF$ | 0.13 | 3.07 | 96.8 | 3.4 | 1.9 |
| 1,2,3,4,7,8,9-$H_pCDF$ | 0.12 | 5.34 | 94.5 | 0.34 | 0.14 |
| OCDF | 1.26 | 26.4 | 72.3 | 0.12 | 2.0 |
| Σi-TE | - | - | - | 1.3 | 0.86 |

[a] "observed" concentrations in ng $kg^{-1}$ dw reported by Kjeller *et al* (1991) for a sample of bulked herbage for the period 1979-1988 taken from Rothamsted, UK

[b] concentration reported for 1,2,3,4,8-/1,2,3,7,8-$P_eCDF$

[c] concentration reported for 1,2,3,4,7,9-/1,2,3,4,7,8-$H_xCDF$

**Table 3: Comparison of "Observed" Foodstuff Concentrations with those Predicted by Model**

| Congener | Predicted $C_{rm}$ | Observed[a] $C_{rm}$ | Predicted $C_{ml}$ | Observed[b] $C_{ml}$ | Predicted $C_c$ | Observed[c] $C_c$ | Predicted $C_{eb}$ | Observed[d] $C_{eb}$ |
|---|---|---|---|---|---|---|---|---|
| 2,3,7,8-TCDD | 0.013 | 0.050 | 0.005 | 0.02 | 0.019 | 0.10 | 0.025 | 0.05 |
| 1,2,3,7,8-$P_eCDD$ | 0.150 | 0.048 | 0.054 | 0.02 | 0.214 | 0.10 | 0.073 | 0.075 |
| 1,2,3,4,7,8-$H_xCDD$ | 0.053 | 0.103[e] | 0.019 | 0.025[e] | 0.120 | 0.635[e] | 0.061 | 0.128[e] |
| 1,2,3,6,7,8-$H_xCDD$ | 0.021 | 0.103[e] | 0.021 | 0.025[e] | 0.142 | 0.635[e] | 0.067 | 0.128[e] |
| 1,2,3,7,8,9-$H_xCDD$ | 0.014 | 0.038 | 0.014 | 0.01 | 0.061 | 0.09 | 0.037 | 0.055 |
| 1,2,3,4,6,7,8-$H_pCDD$ | 0.057 | 1.7 | 0.021 | 0.09 | 0.210 | 2.5 | 0.264 | 0.845 |
| OCDD | 0.487 | 16.5 | 0.172 | 0.52 | 0.208 | 3.5 | 0.706 | 3.8 |
| 2,3,7,8-TCDF | 0.506 | 0.105 | 0.184 | 0.005 | 2.60 | 0.185 | 0.392 | 0.105 |
| 1,2,3,7,8-$P_eCDF$ | 0.053 | 0.013 | 0.019 | 0.005 | 0.296 | 0.035 | 0.407 | 0.02 |
| 2,3,4,7,8-$P_eCDF$ | 0.160 | 0.105 | 0.056 | 0.03 | 0.330 | 0.065 | 0.203 | 0.075 |
| 1,2,3,4,7,8-$H_xCDF$ | 0.068 | 0.10 | 0.021 | 0.01 | 0.134 | 0.07 | 0.082 | 0.065 |
| 1,2,3,7,8,9-$H_xCDF$ | 0.047 | 0.36[f] | 0.002 | 0.005 | 0.005 | -[g] | 0.0085 | 0.005 |
| 1,2,3,6,7,8-$H_xCDF$ | 0.033 | 0.050 | 0.012 | 0.01 | 0.077 | 0.04 | 0.049 | 0.035 |
| 2,3,4,6,7,8-$H_xCDF$ | 0.025 | 0.020 | 0.008 | 0.005 | 0.032 | 0.035 | 0.012 | 0.03 |
| 1,2,3,4,6,7,8-$H_pCDF$ | 0.127 | 0.220 | 0.043 | 0.03 | 0.323 | 1.11 | 0.361 | 0.11 |
| 1,2,3,4,7,8,9-$H_pCDF$ | 0.033 | 0.030 | 0.012 | 0.005 | 0.029 | 0.06 | 0.026 | -[g] |
| OCDF | 0.007 | 2.65 | 0.002 | 0.035 | 0.017 | 0.515 | 0.017 | 0.04 |
| Σi-TE | 0.252 | 0.254 | 0.090 | 0.057 | 0.630 | 0.399 | 0.262 | 0.194 |

[a] concentrations quoted are the mean of 2 samples of "meat products" reported by MAFF[6]. Where concentration was reported as <LOD, value quoted is LOD/2

[b] quoted concentrations are the mean of retail milk sampled in summer from 7 UK locations by MAFF[6]

[c] levels cited are the mean of two "poultry" samples reported by MAFF[6]

[d] concentrations quoted are the mean of two "egg" samples reported by MAFF[6]

[e] level reported as 1,2,3,4,7,8-/1,2,3,6,7,8-HxCDD by MAFF[6], values used here assume this level to comprise equal amounts of both congeners

[f] value reported is for one sample only

[g] concentration reported as "not available" by MAFF[6]