Challenges in the modelling of plant uptake of organic pollutants

Modelling the exposure of children and adults to chemicals in the environment

- Crop-specific models
  - Roots (Carrot model)
  - Tubers (Potato model)
  - Leafy vegetables (Lettuce model)
  - Fruits (Tree fruit model)
- Application of models
  - Estimating dietary intakes
  - Comparison to TGD

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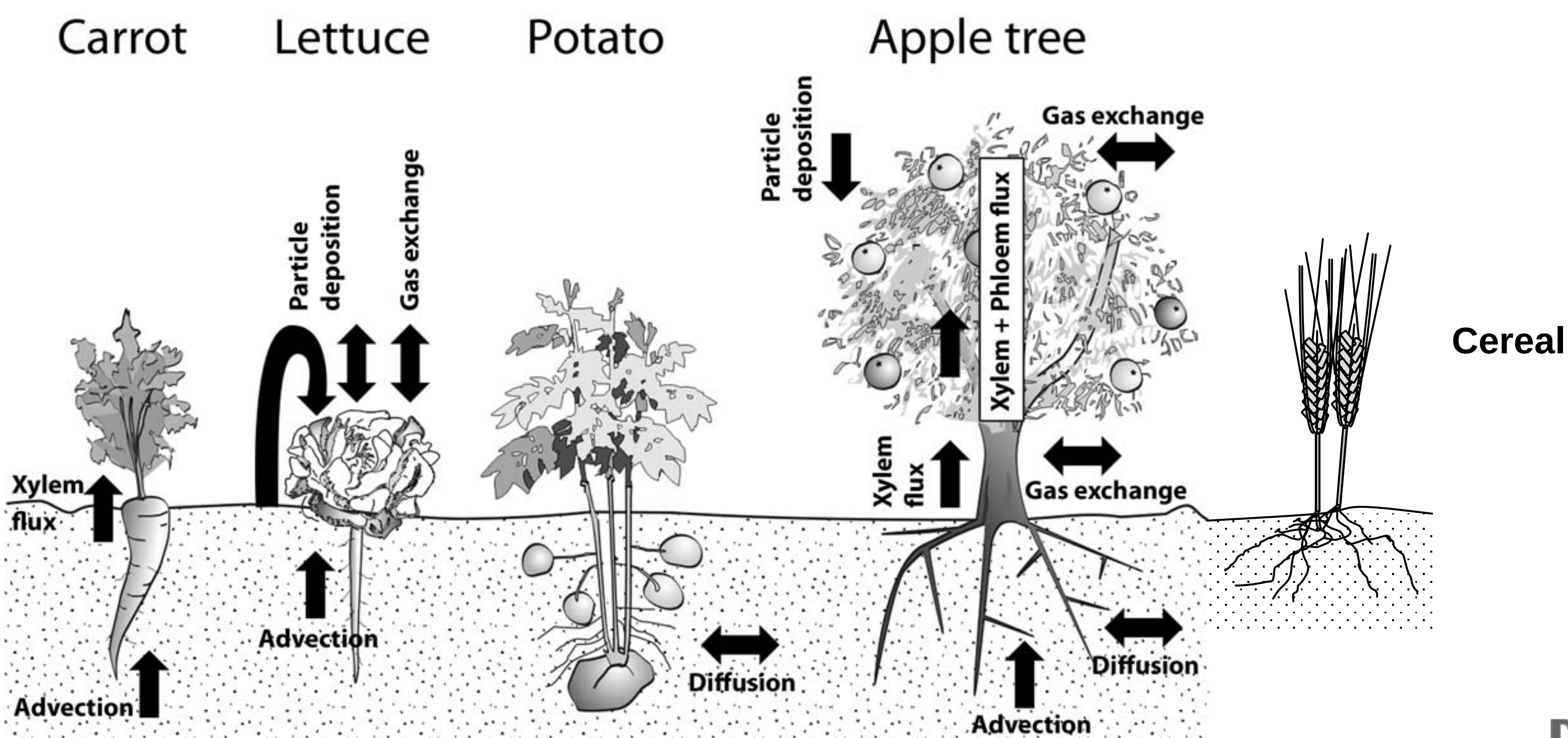
Charlotte Legind - CV

- MSc in Environmental Chemistry (University of Copenhagen)
- PhD student (National Environmental Research Institute, University of Copenhagen, Technical University of Denmark)
- Topic: Uptake of organic chemicals in plants

Overview of crop specific models



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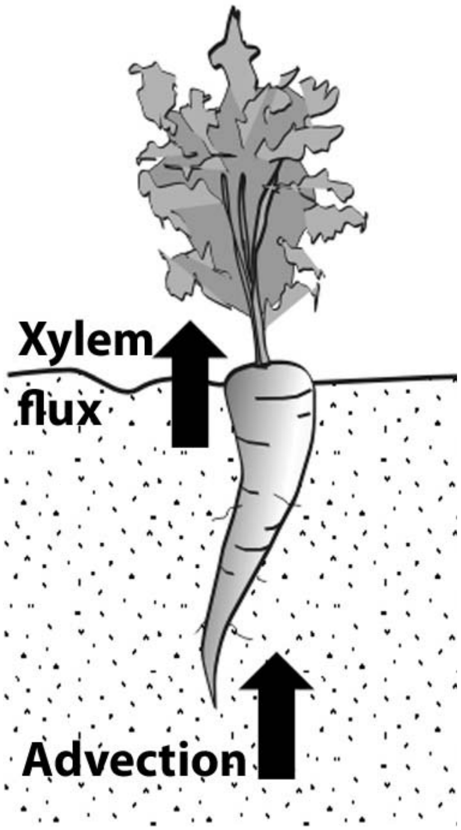
(Models: Trapp (95, 02, and 07) and Travis & Arms (88))

Carrot model (only advection)



$$\frac{dC_R}{dt} = C_S \cdot K_{WS} \cdot Q/M - C_{XY} \cdot Q/M - k \cdot C_R$$

$$C_{XY} = C_R / K_{RW}$$

Steady state solution

$$C_R = \frac{Q}{Q/K_{RW} + k \cdot M} \cdot K_{WS} \cdot C_S$$

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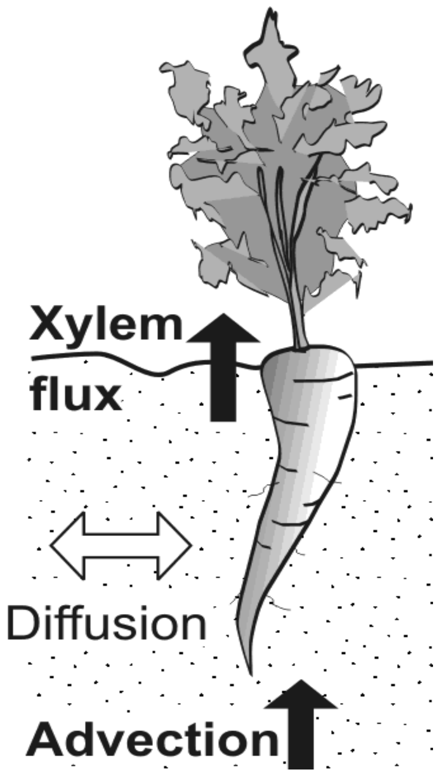
Trapp, S., Environ. Toxicol. Chem., 2002, 21, 203-206

Carrot model (with diffusion)



$$\frac{dC_R}{dt} = C_S \cdot K_{WS} \cdot Q/M - C_{XY} \cdot Q/M - k \cdot C_R + \frac{A \cdot P \cdot 1000}{M}(C_S \cdot K_{WS} - C_{XY})$$

Steady state solution

$$C_R = \frac{(Q + 1000 \cdot A \cdot P)}{\frac{Q + 1000 \cdot A \cdot P}{K_{RW}} + k \cdot M} \cdot K_{WS} \cdot C_S$$

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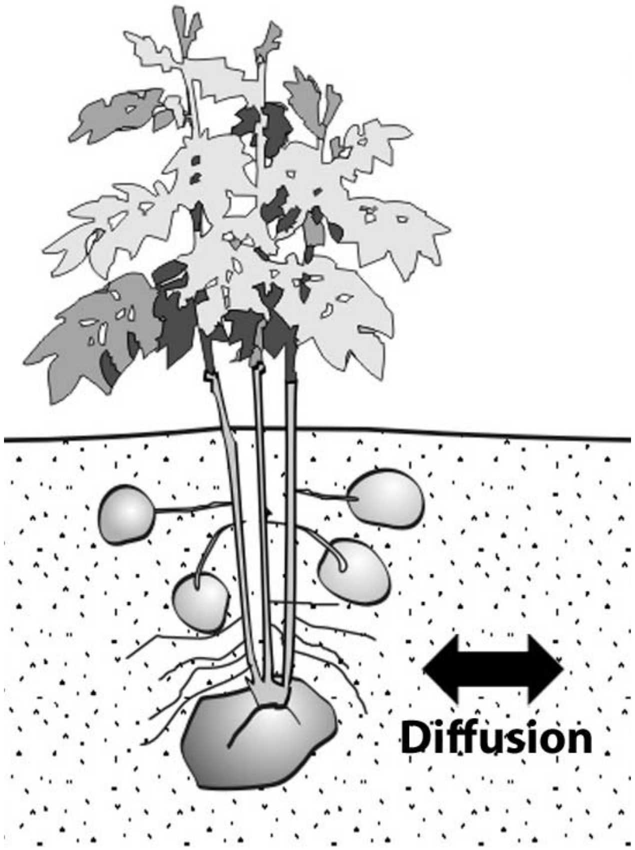
Trapp, S., SAR QSAR Environ. Res., 2007, 18, 367-387

Potato model



$$\frac{dC_P}{dt} = k_{Uptake} \cdot C_S - k_{Loss} \cdot C_P$$

Steady state solution

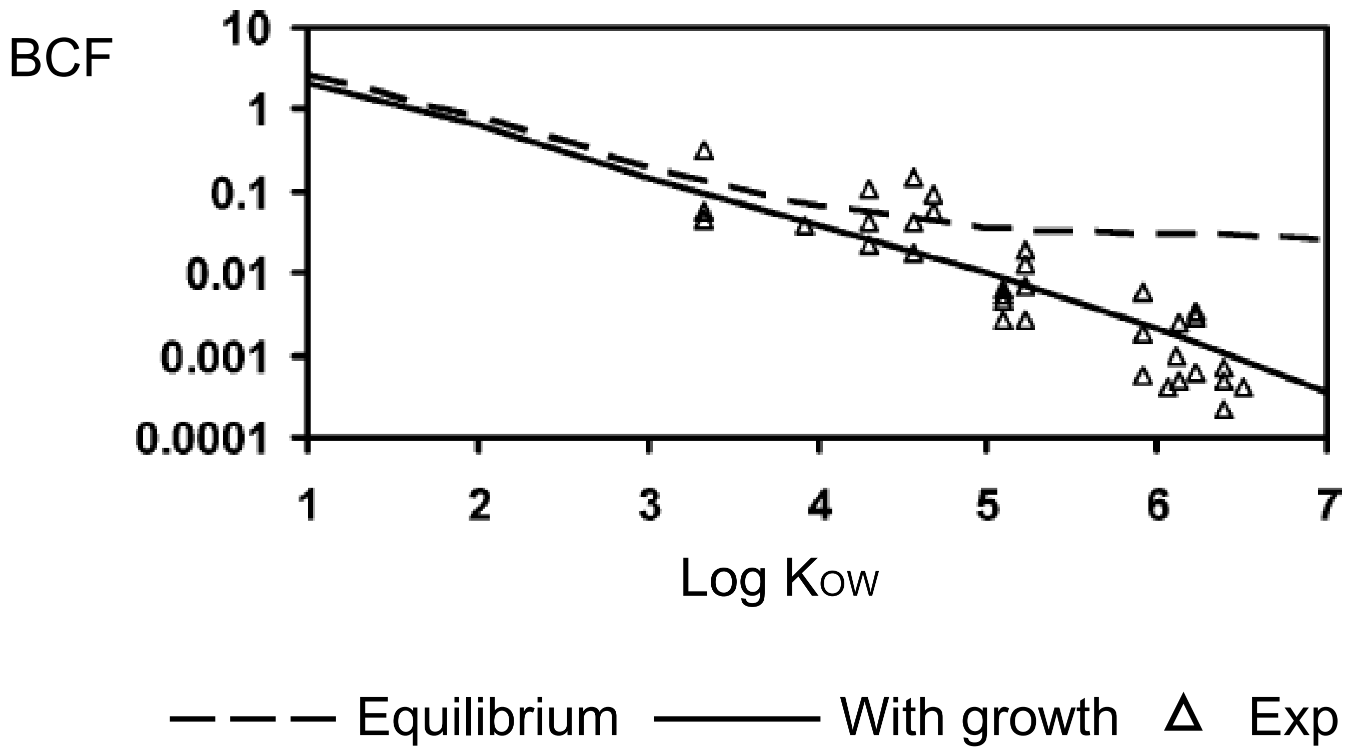
$$BCF = \frac{k_{Uptake}}{k_{Loss}} = \frac{C_P}{C_S} = \frac{K_{PW}}{K_{SW}}$$

$$k_{Loss} = \frac{23 \cdot D_P}{R^2} \qquad k_{Uptake} = k_{Loss} \cdot BCF$$

$$BCF^* = \frac{k_{Uptake}}{k_{Loss} + k_{Growth}}$$

Trapp, S. et al., Environ. Sci. Technol., 2007, 41, 3103-3108

+/- growth dilution



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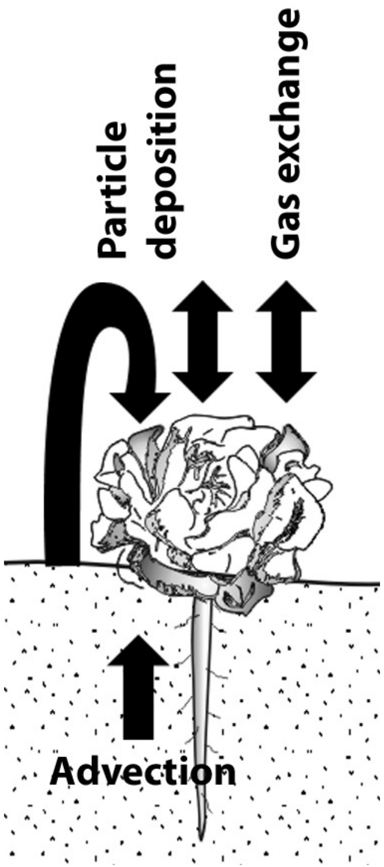
Trapp, S. et al., Environ. Sci. Technol., 2007, 41, 3103-3108

Lettuce model



$$\frac{dC_L}{dt} = b - a \cdot C_L \qquad a = \frac{A \cdot g_L}{M \cdot K_{LA}} + k$$

$$b = \frac{Q}{M} \cdot TSCF \cdot C_S \cdot K_{WS}$$

$$+ \frac{A}{M} \cdot C_{A,t} \left(g_L (1 - f_P) + \frac{U_{dep}}{2} \cdot f_P \right)$$

Steady state solution

$$C_L(\infty) = \frac{b}{a}$$

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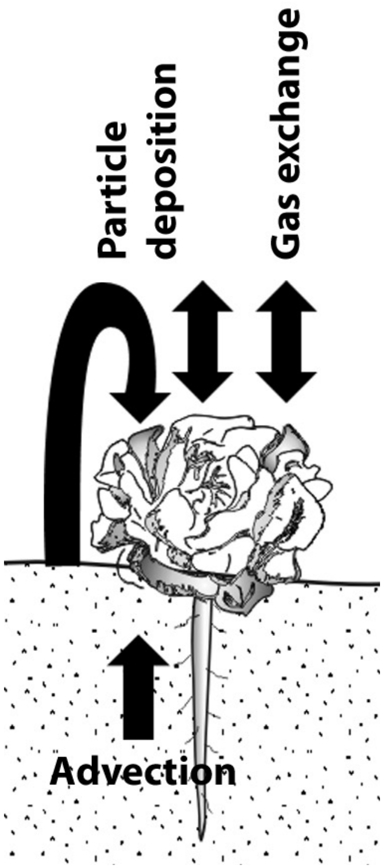
Trapp, S. & Matthies, M., Environ. Sci. Technol., 1995, 29, 2333-2338

Lettuce model



Growth period of 60 days

$$C_L(t) = C_L(0) \cdot e^{-a \cdot t} + \frac{b}{a}(1 - e^{-a \cdot t})$$

Attached soil: 1% (ww)

$$BCF\,with\,soil = BCF\,model + 0.01$$

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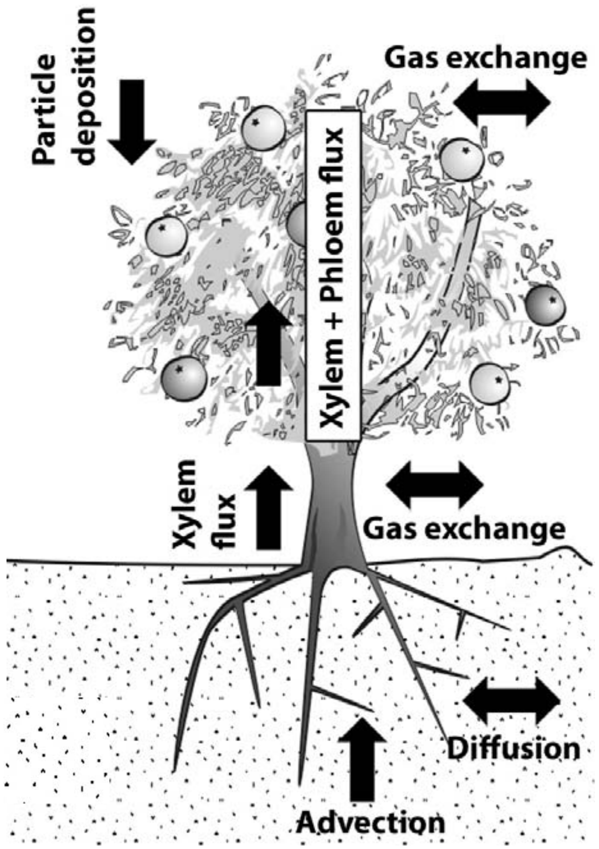
Trapp, S. & Matthies, M., Environ. Sci. Technol., 1995, 29, 2333-2338

Tree fruit model



Eight compartments:

- Fine roots
- Thick roots
- Stem
- Leaves
- Fruits ←
- Soil 1 & 2
- Air

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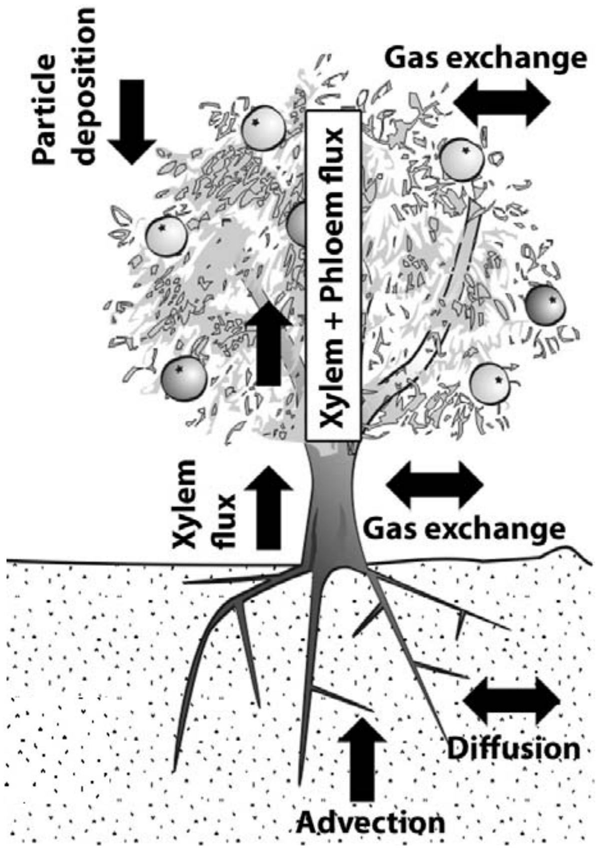
Trapp, S., SAR QSAR Environ. Res., 2007, 18, 367-387

Tree fruit model



$$\frac{dC_F}{dt} = \frac{A}{M} \cdot C_{A,t}\left(\frac{P_F}{K_{AW}}(1-f_P) + \frac{U_{dep}}{2} \cdot f_P\right) + \frac{Q}{M} \cdot C_{XY} - \frac{1000 \cdot A \cdot P_F}{K_{FW} \cdot M} \cdot C_F - k \cdot C_F$$

Steady state solution

$$C_F = \frac{A \cdot C_{A,t}\left(\frac{P_F}{K_{AW}}(1-f_P) + \frac{U_{dep}}{2} \cdot f_P\right) + Q \cdot C_{XY}}{\frac{1000 \cdot A \cdot P_F}{K_{FW}} + k \cdot M}$$

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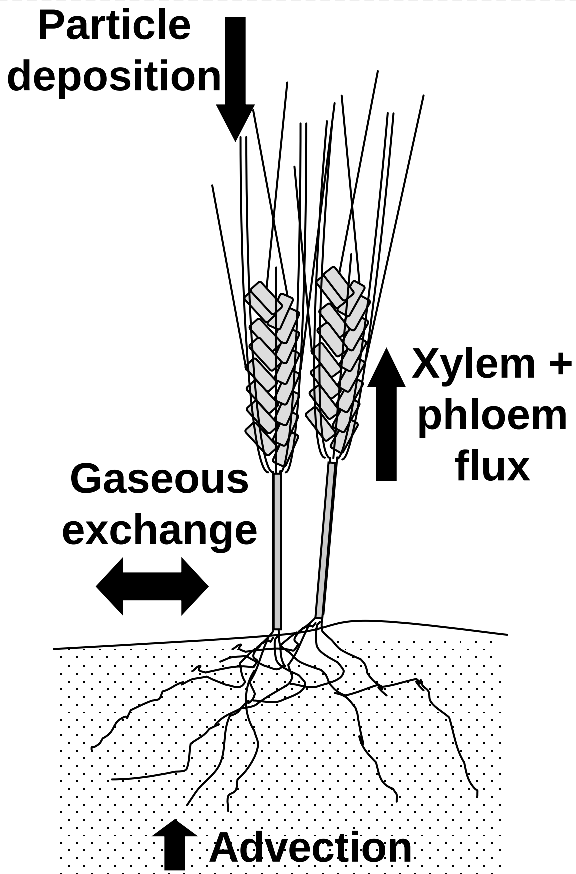
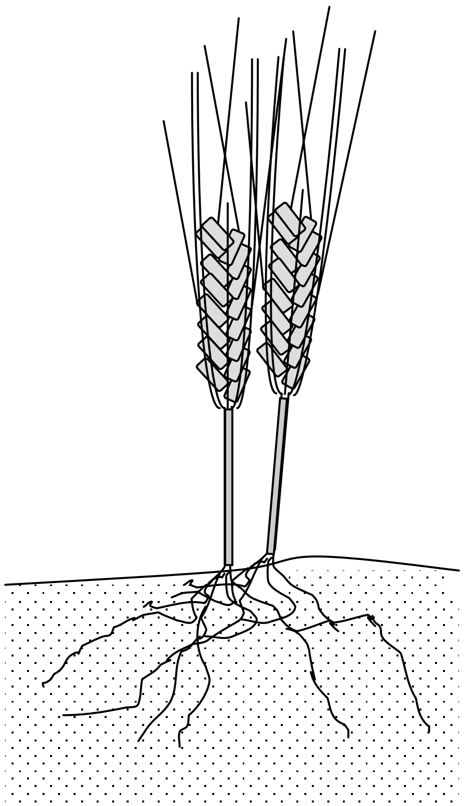
Trapp, S., SAR QSAR Environ. Res., 2007, 18, 367-387

Cereal model ?



- Currently no valid model for cereal
- Could be similar to the fruit tree model
- Needs measured data

Cereal model ?



Regression for vegetation

$$BCFveg = \frac{C_{veg}}{C_S}$$

$$\text{Log}\,BCFveg = 1.588 - 0.578 \cdot \log K_{OW}$$

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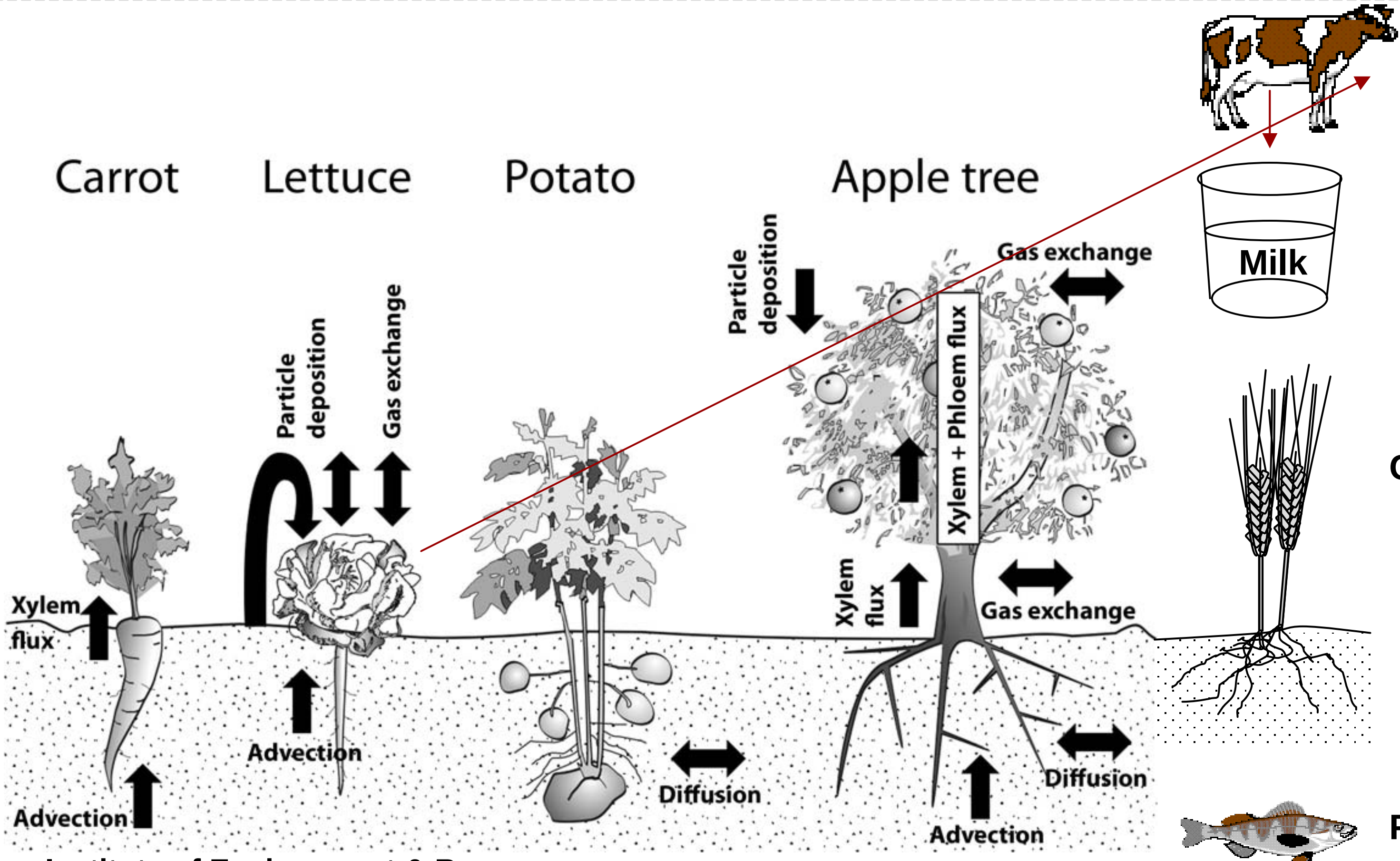
Travis, C.C. & Arms, A.D., Environ. Sci. Technol., 1988, 22, 271-274

Application of models

- Determine exposure to environmental pollutants through diet, drinking water, soil ingestion, and air inhalation
- Determine exposure to environmental pollutants through crops only
- Compare the model framework (NMF) to current risk assessment approaches in the EU (TGD) and measured estimates

New model framework (NMF)
Crops only and total diet



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(Models: Trapp (95, 02, and 07), Travis & Arms (88), and TGD (03))

Consumption data (DK and TGD)

Crops

(40-60% of total consump tion)

Food type	4-13		14-75 (♀)		TGD
	Mean	95th	Mean	95th	
Root vegetables (g/d)	33	65	43	89	384
Potatoes (g/d)	73	165	90	198	
Lettuce (g/d)	7	13	9	18	1200
Other leafy veg. (g/d)	8	15	10	21	
Tree fruits (g/d)	127	278	137	318	
Cereal products (g/d)	205	308	195	309	
Milk (g/d)	500	950	303	754	561
Meat (g/d)	109	221	113	231	301
Fish (g/d)	12	39	17	47	115
Inhalation (m^3/d)	10.7	28.8	11.3	38.4	20 x 0.75
Soil ingestion (mg/d)	100	200	50	300	0
Drinking water (L/d)	0.9	1.75	1.4	2.3	2
Bodyweight (kg)	35.1		67.3		70

Danskernes Kostvaner 2000-2002, Lyhne et al. 2005, Danmarks Fødevareforskning
Pesticides Food Monitoring, 1998-2003, Part 2, Poulsen et al. 2005, Danish Veterinary and Food Administration

Input concentrations in soil, air, and water

(BaP, TCDD: background
LAS: sewage sludge application)

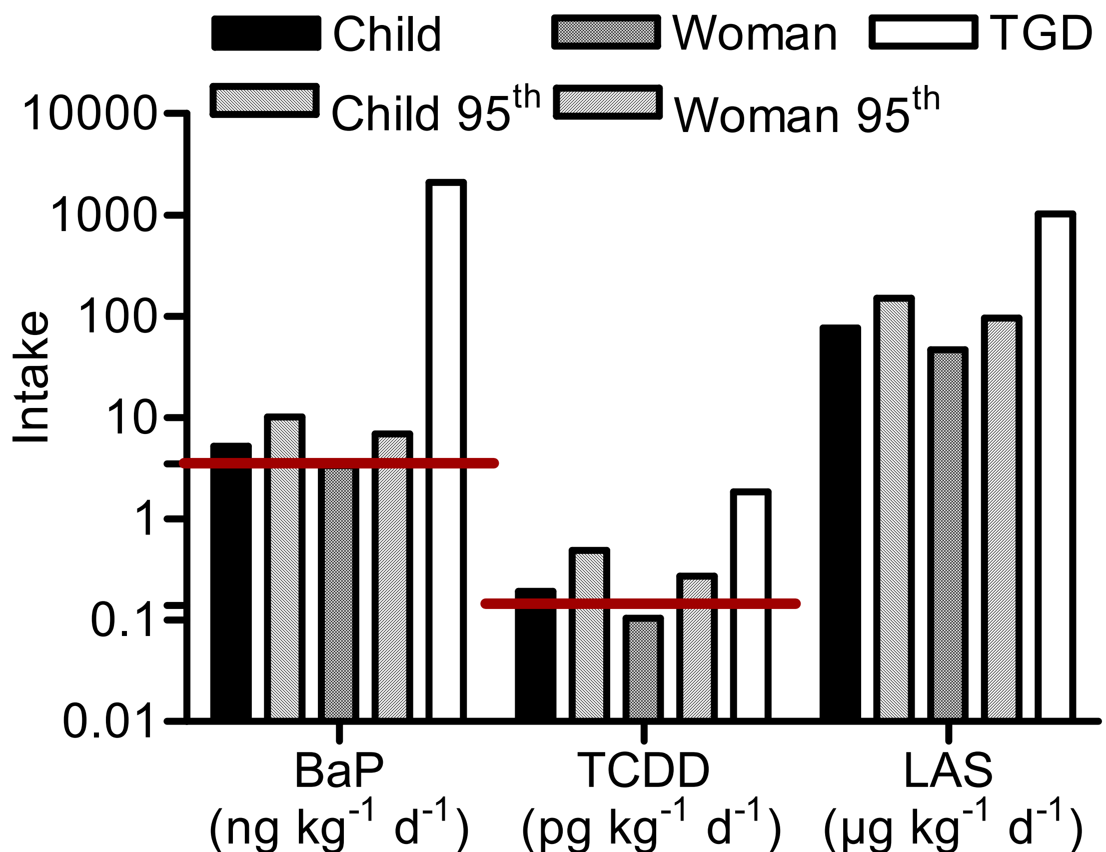
Symbol	BaP	TCDD	LAS
C_S (mg/kg ww)	0.069	$4.02 \cdot 10^{-8}$	4.1
C_A (µg/m^3)	0.001	$1.7 \cdot 10^{-9}$	0
C_W (µg/L)	0.023	$5.61 \cdot 10^{-9}$	27

Daily intake

$$DDI = \frac{\sum_i (C_i \cdot Consumption_i)}{Bodyweight}$$

Measured (—) vs. modelled daily intakes
Total consumption

Total consumption



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Measured (—, total) vs. modelled daily intakes (crops only)

Crops only

<u>BaP</u>

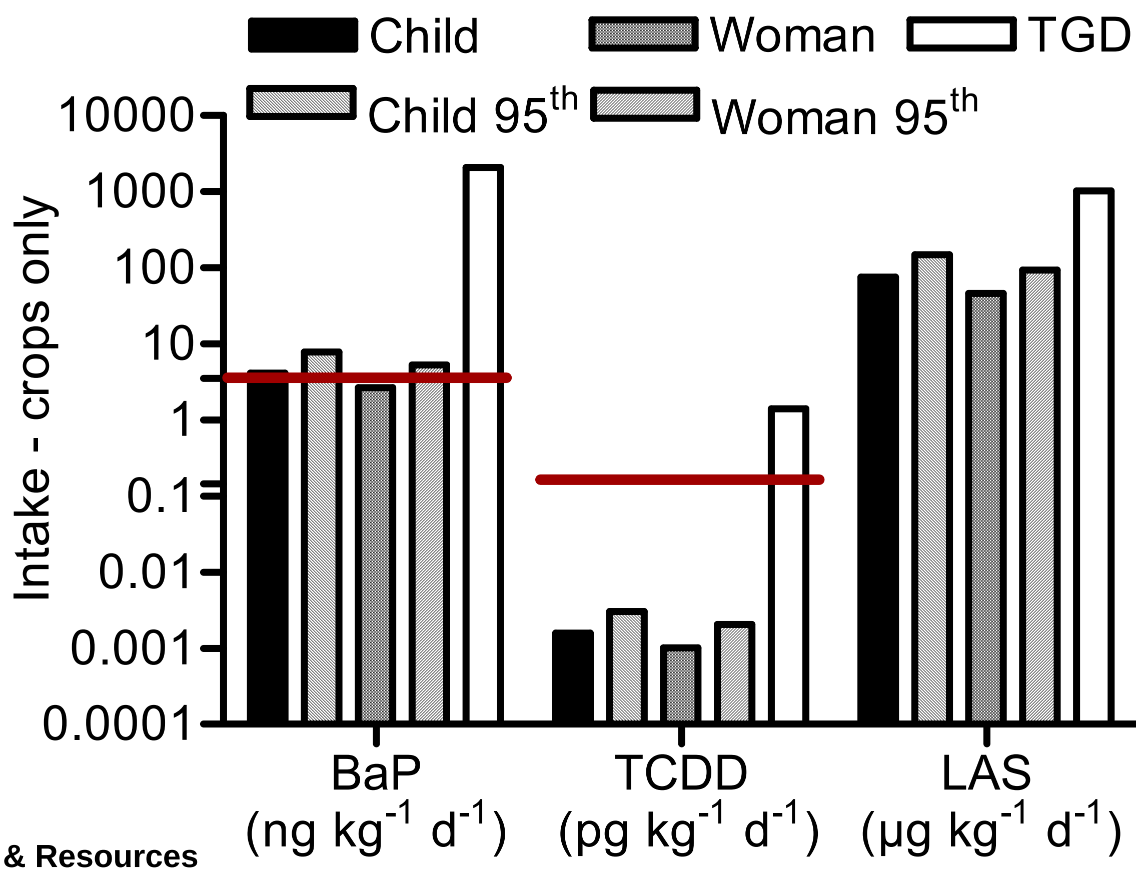
NMF: 76-79%
TGD: 100%

<u>TCDD</u>

NMF: 1%
TGD: 76%

<u>LAS</u>

NMF: 99%
TGD: 100%



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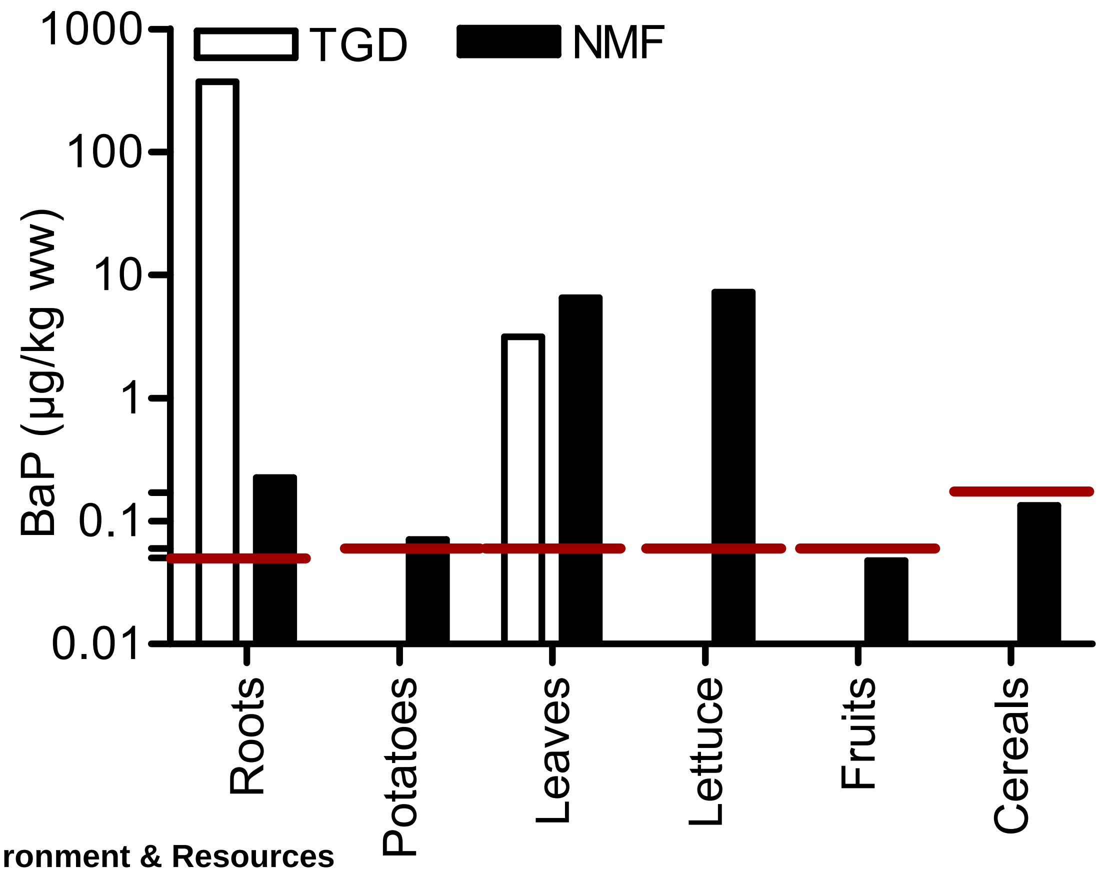
Measured (—) vs. modelled concentrations in different food stuffs - BaP



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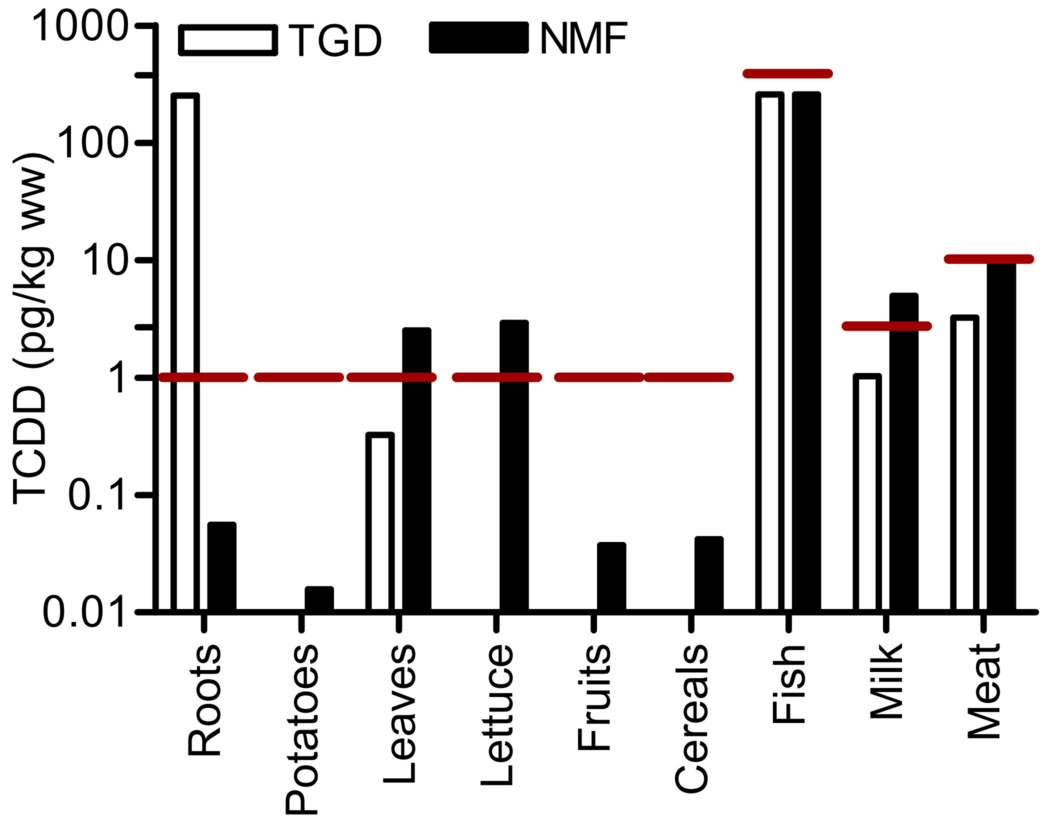
Measured (—) vs. modelled concentrations in different food stuffs - TCDD



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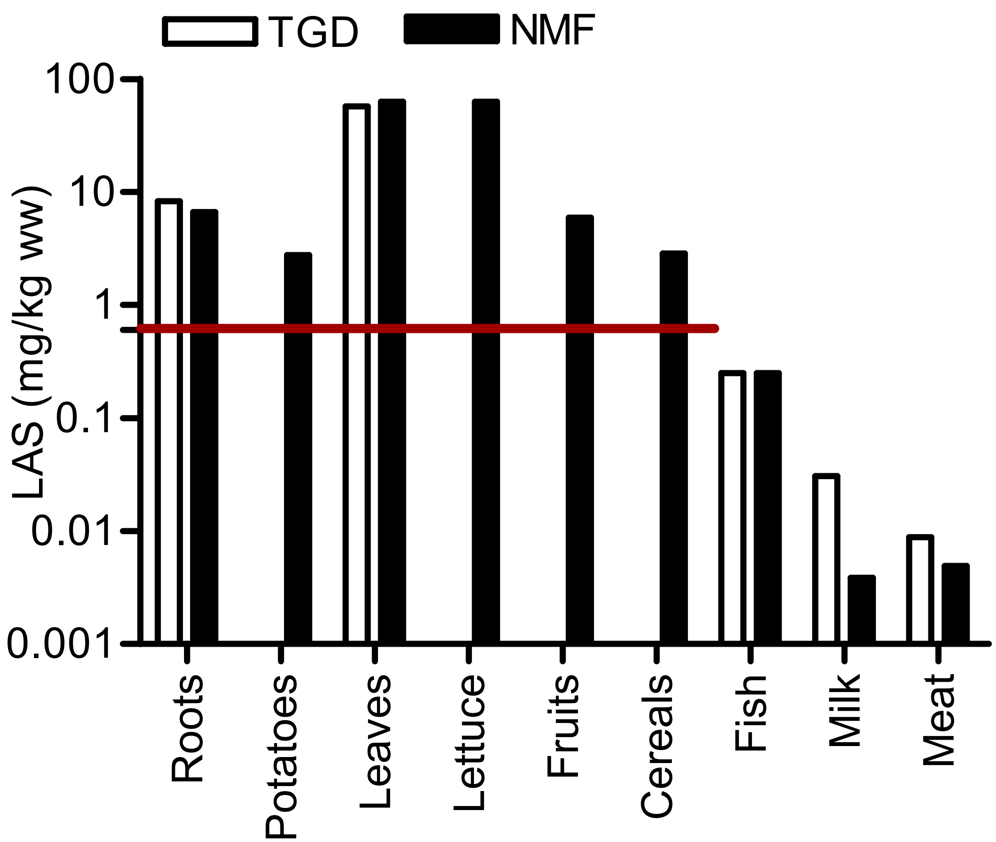
Measured (—) vs. modelled concentrations in different food stuffs - LAS



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Sources of environmental pollutants in the diet

	BaP			TCDD			LAS		
%	TGD	4-13	14-75	TGD	4-13	14-75	TGD	4-13	14-75
Total diet									
Soil source	97	28	23	76	-	-	100	99	99
Air source	-	61	63	-	53	38	-	-	-
Water source	-	11	14	23	46	62	-	1	1
Crops only									
Soil source	97	31	27	100	26	23	100	100	100
Air source	3	69	73	-	74	77	-	-	-

Based on background concentrations in soil, air, and water

$C_A = C_W = 0$ =>
Acceptable soil concentration:
ASC = TDI/intake x C_S

Most important food stuffs - total diet

%	BaP			TCDD			LAS		
	TGD	4-13	14-75	TGD	4-13	14-75	TGD	4-13	14-75
Soil ingestion	-	4	2	-	-	-	-	-	-
Inhalation	-	6	5	-	-	-	-	-	-
Drinking water	-	11	14	-	-	-	-	1	1
Roots	97	4	4	75	-	-	4	8	9
Potatoes	-	3	3	-	-	-	-	7	8
Leaf veg.	3	27	29	-	-	-	95	18	20
Lettuce	-	27	28	-	-	-	-	16	18
Fruits	-	3	3	-	-	-	-	28	26
Fish	-	-	-	23	46	62	38-55%	-	-
Milk	-	-	-	-	37	21	30-40%	-	-
Meat	-	-	-	1	16	15	13-18%	-	-
Cereal	-	15	12	-	-	-	-	22	18

Most important food stuffs
Crops only

%	BaP			TCDD			LAS		
	TGD	4-13	14-75	TGD	4-13	14-75	TGD	4-13	14-75
Roots	97	5	6	100	3	4	4	8	9
Potatoes	-	4	4	-	2	2	-	8	8
Leaf veg.	3	35	37	-	35	37	96	18	21
Lettuce	-	34	36	-	36	38	-	16	18
Fruits	-	4	4	-	9	7	-	28	26
Cereal	-	19	15	-	16	12	-	22	18

Conclusions

- Crop-specific models are available for roots, tubers, leafy vegetables, and tree fruits
- Measured data are needed to develop a cereal model
- The NMF comes close to measured estimates of dietary intakes
- The NMF offers more details concerning which food stuffs are important for dietary intakes of pollutants. This information may be relevant for risk management.
- Children should be included in risk assessment

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- Jens Streibig for PhD supervision