The field as a unit process

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PESTLCI

– a model estimating pesticide emissions for LCA of agricultural products

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Technical University of Denmark

Life Cycle Impact Assessment of Pesticides
19th Discussion Forum on Life Cycle Assessment
ETH Zürich 27 March 2003

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Pesticide emission inventory for field processes

- The need
- The modular framework
- The modules of PESTLCI
- The results
- The further work

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The need behind PESTLCI

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LCI of field crops

Known:

- Quantity and identity of applied pesticide
- Crop type and application technique
- Meteorological and pedological conditions

Wanted:

- Inventory of pesticide emissions to the environment, air, soil, surface water and groundwater
- Based on generally available substance data

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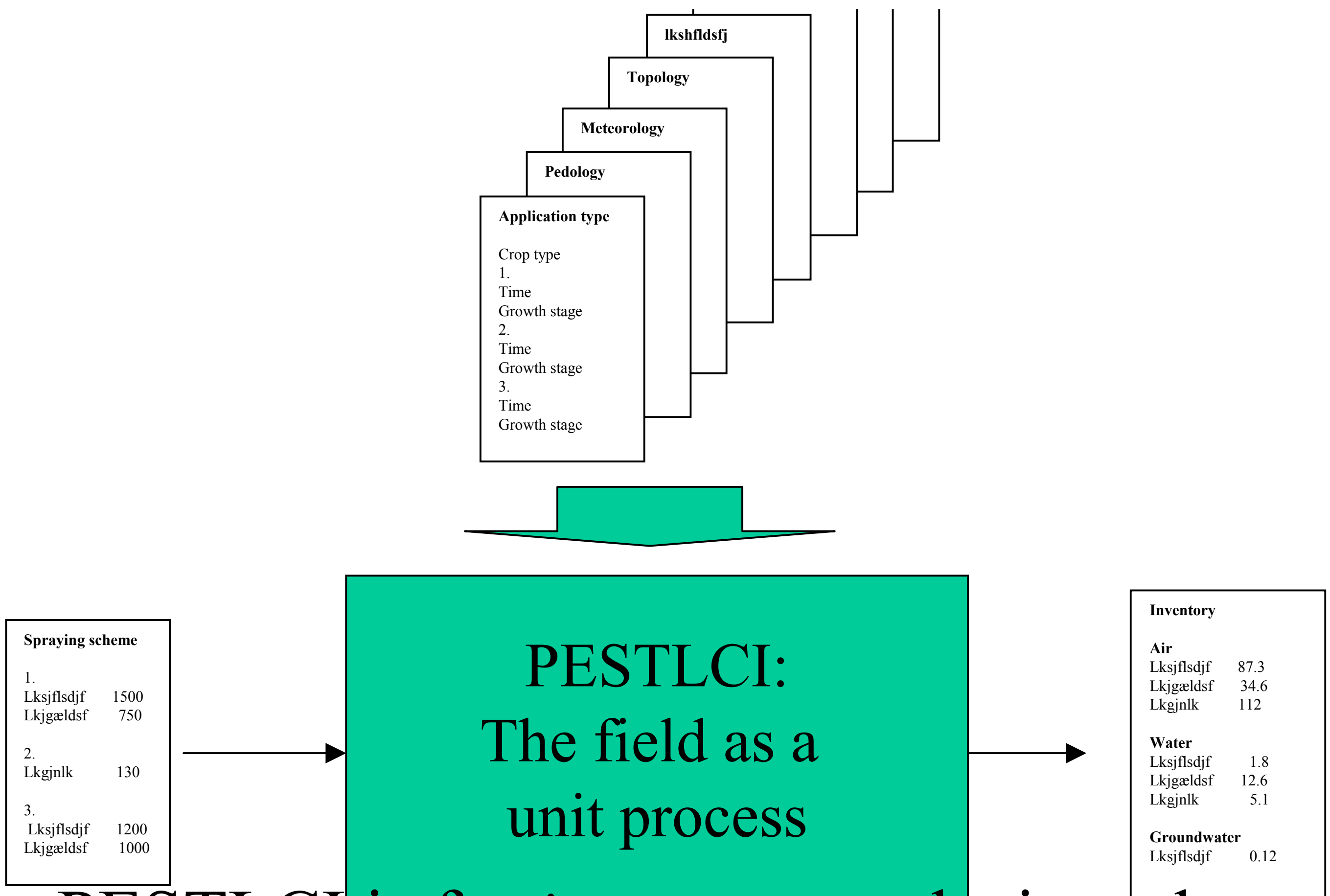
The need



PESTLCI is for *inventory* analysis, to be combined with LCIA method of own choice

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The environment

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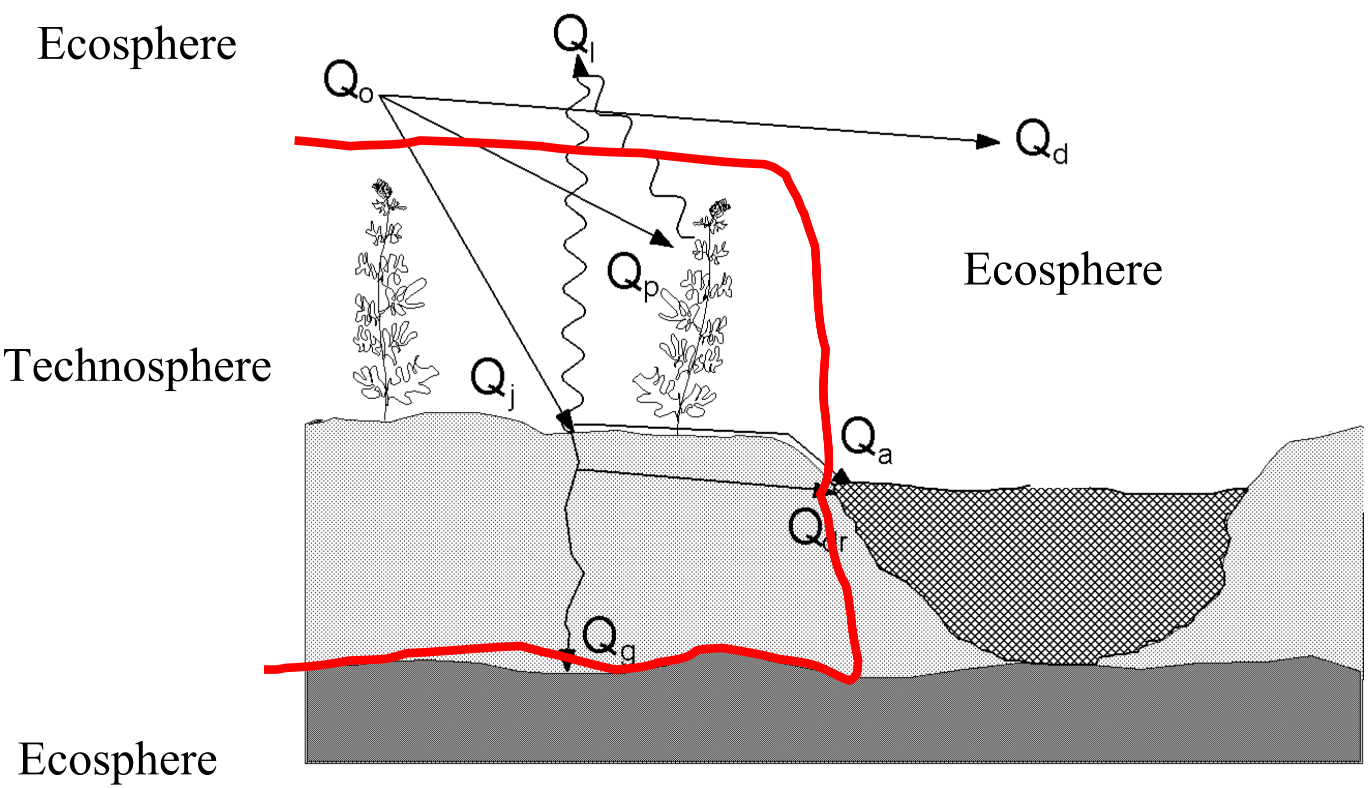
The field is seen as a part of the technosphere

- Emission means crossing the boundary to the ecosphere



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The framework for PESTLCI

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Modular approach;

- Individual modules for distinct fate processes in the field system,
  - combined through fractions emitted or degraded
- Transparency
- Flexibility to updating
- Flexibility to adaptation
- Facility to calibrate and validate against empirical data

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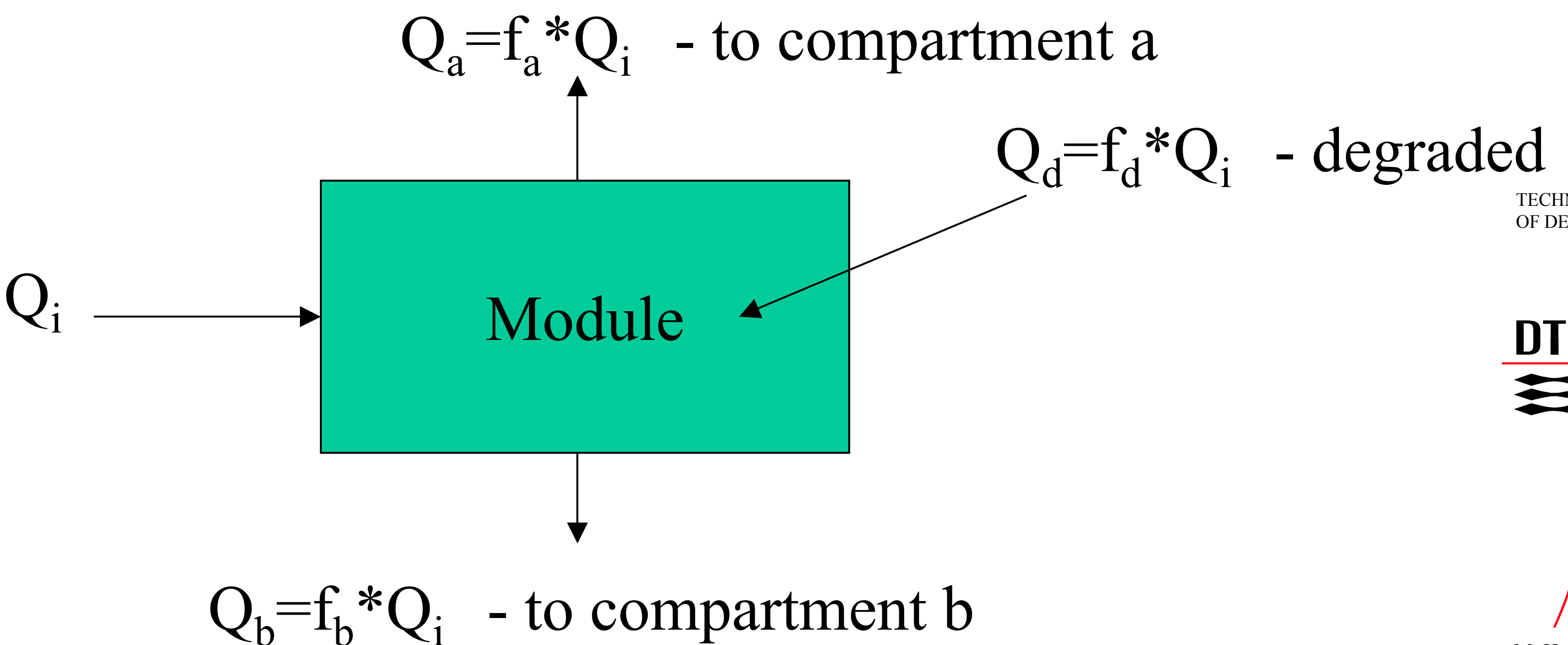
General form of PESTLCI modules

In: Quantity

Out: Fractions undergoing different fates



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M. Hauschild

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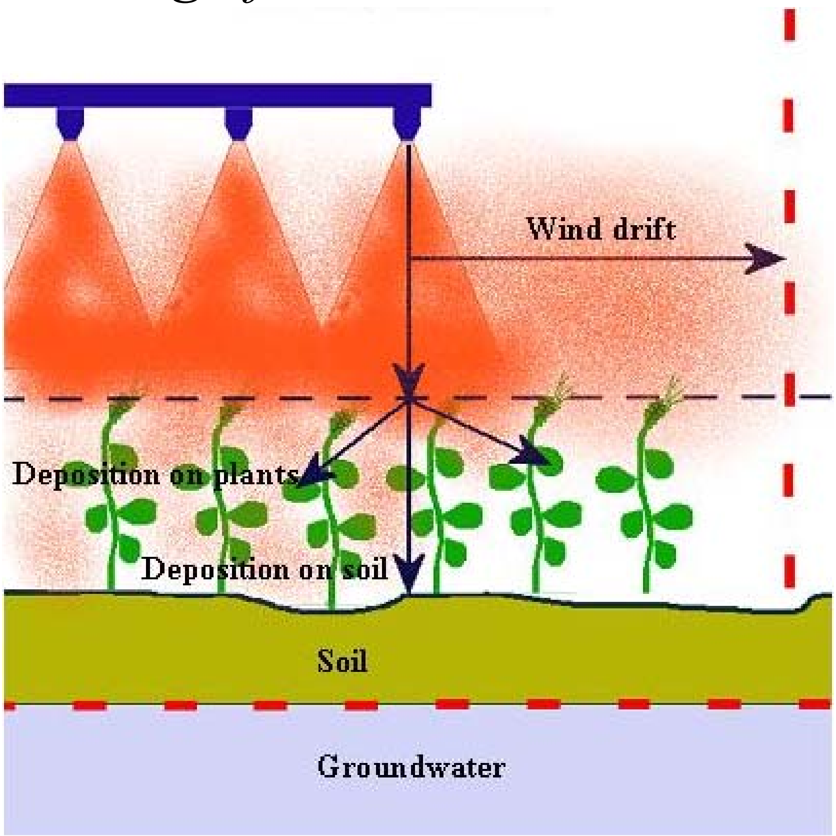
The modules of PESTLCI

Based on own earlier work and review of existing approaches for risk assessment/ranking of pesticides

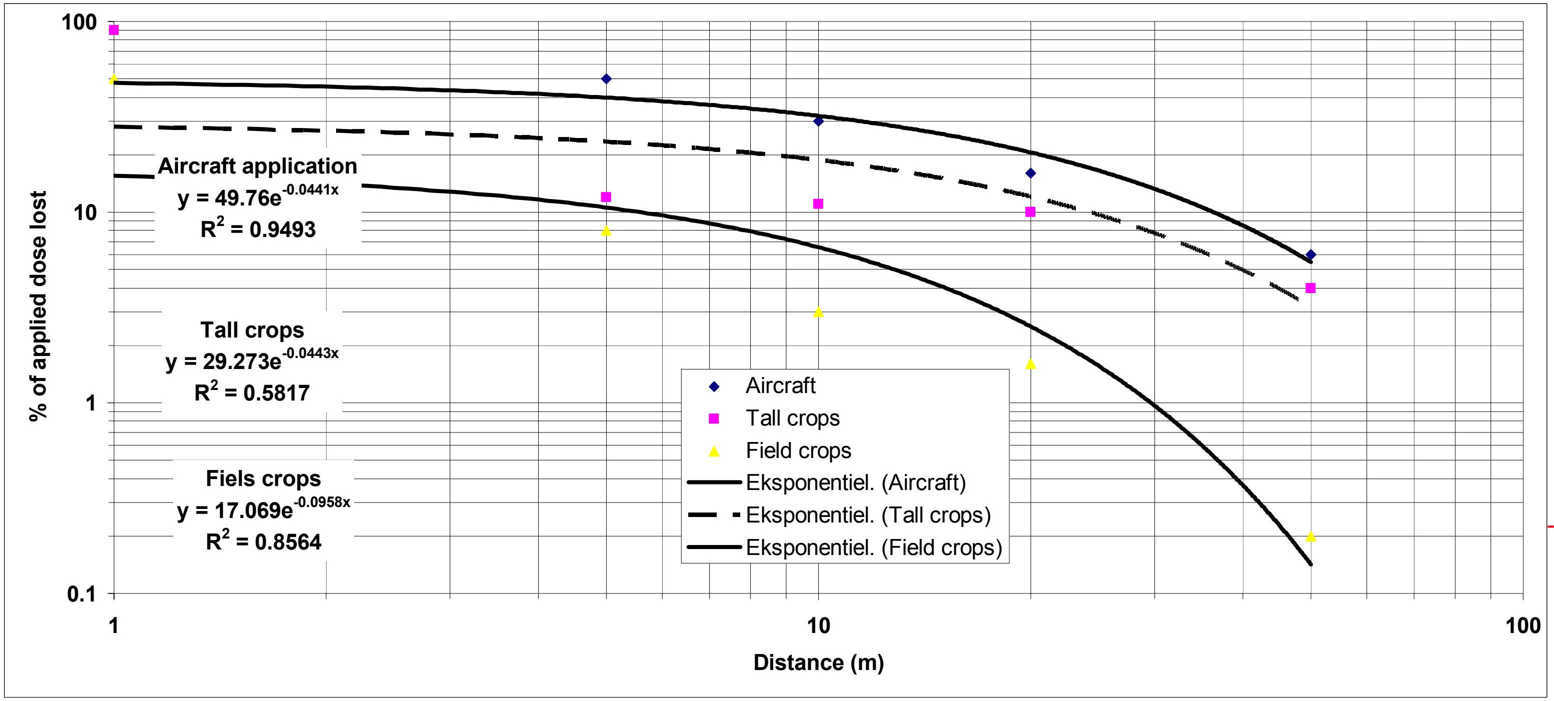


Primary distribution processes

- Immediately after application
  - Drift
  - Distribution between canopy and soil

Wind drift module

Dependence of wind drift loss on distance to field edge and type of application



Wind drift fraction found by integration over entire field

European and Mediterranean Plant Protection Organisation (EPPO), *Council of Europe, 96/5543*

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Interception by canopy

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Default factors for 28 Crops at 2-5 developmental stages

Crop	**Growth phase**	$\mathbf{f_p}$
Bare soil – pre-emergence	Not applicable	0
Beans I	Leaf development	0.25
Beans II	Stem elongation	0.4
Beans III	Flowering	0.7
Beans IV	Ripening/senescence	0.8
Bulbs I	Leaf development/stem elongation I (<=3 weeks after emergence)	0.2
Bulbs II	Leaf development/stem elongation I (3-6 weeks a.e.)	0.6
Bulbs III	Flowering	0.5

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Linders, J., Mensink, H., Stephenson, G., Wauscope, D. & Racke, K. (2000). *Pure Appl. Chem., Vol. 72, No. 11, pp. 2199-2218.*

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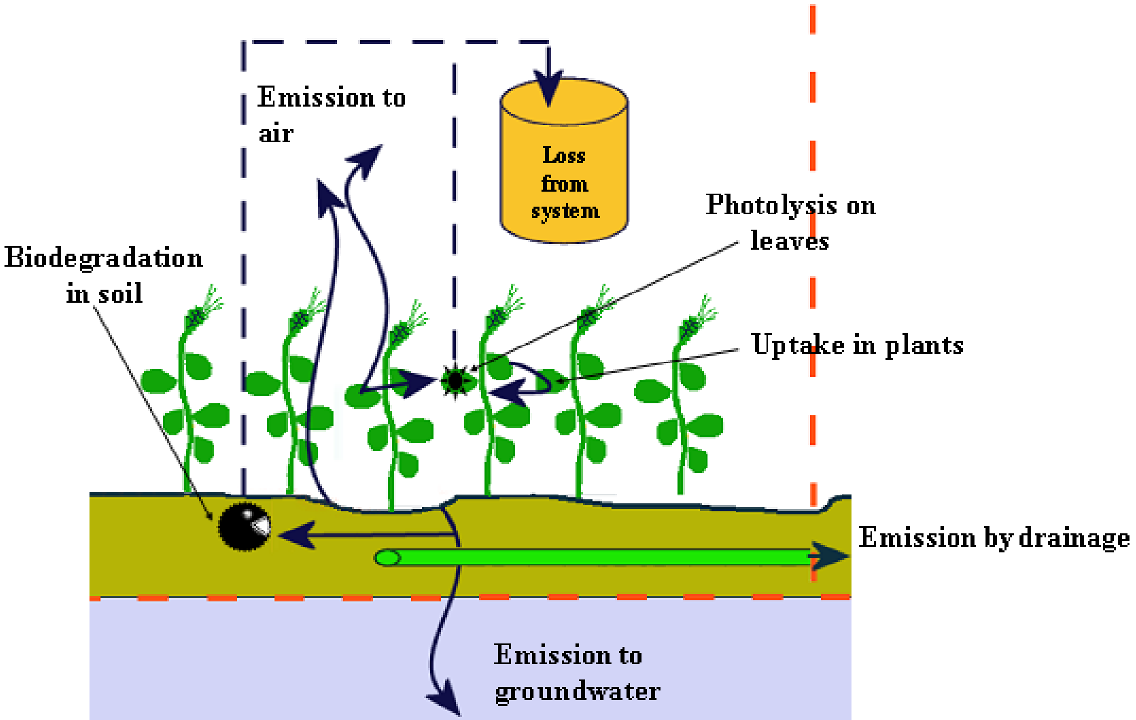
The modules of PESTLCI

Secondary distribution processes

- On leaf
  - Uptake
  - Evaporation
  - Abiotic degradation
- On or in soil
  - Leaching to groundwater or surface water
  - Degradation
  - Run-off
  - Evaporation



Leaf uptake module

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Treated as removal mechanism in PESTLCI

Also of relevance to human exposure in some impact assessment methodologies, but

….. how much reaches the food?

Developed from complex model by Satchivi et al.

- focused on the rate-limiting process, *diffusion across cuticula*
- based on only two parameters:
  - the dissociation-corrected K_{ow} (affinity for cuticula wax)
  - the molecular volume (resistance to diffusion)

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Satchivi, N.M. et al. (2000). *Pesticide Biochemistry and Physiology, Vol. 68, pp. 67-84 and pp. 85-95.*

Leaf uptake module

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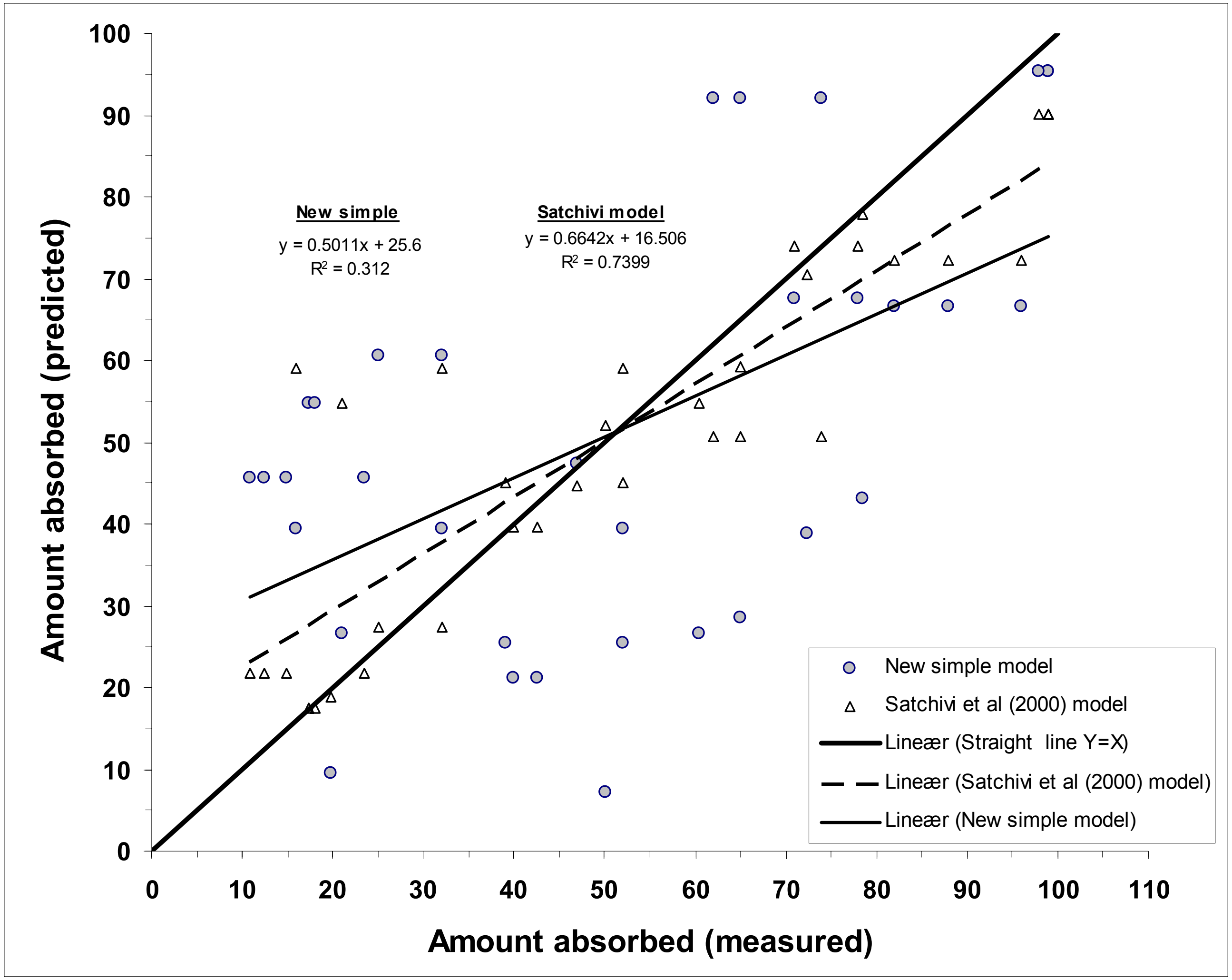

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Evaporation from leaves

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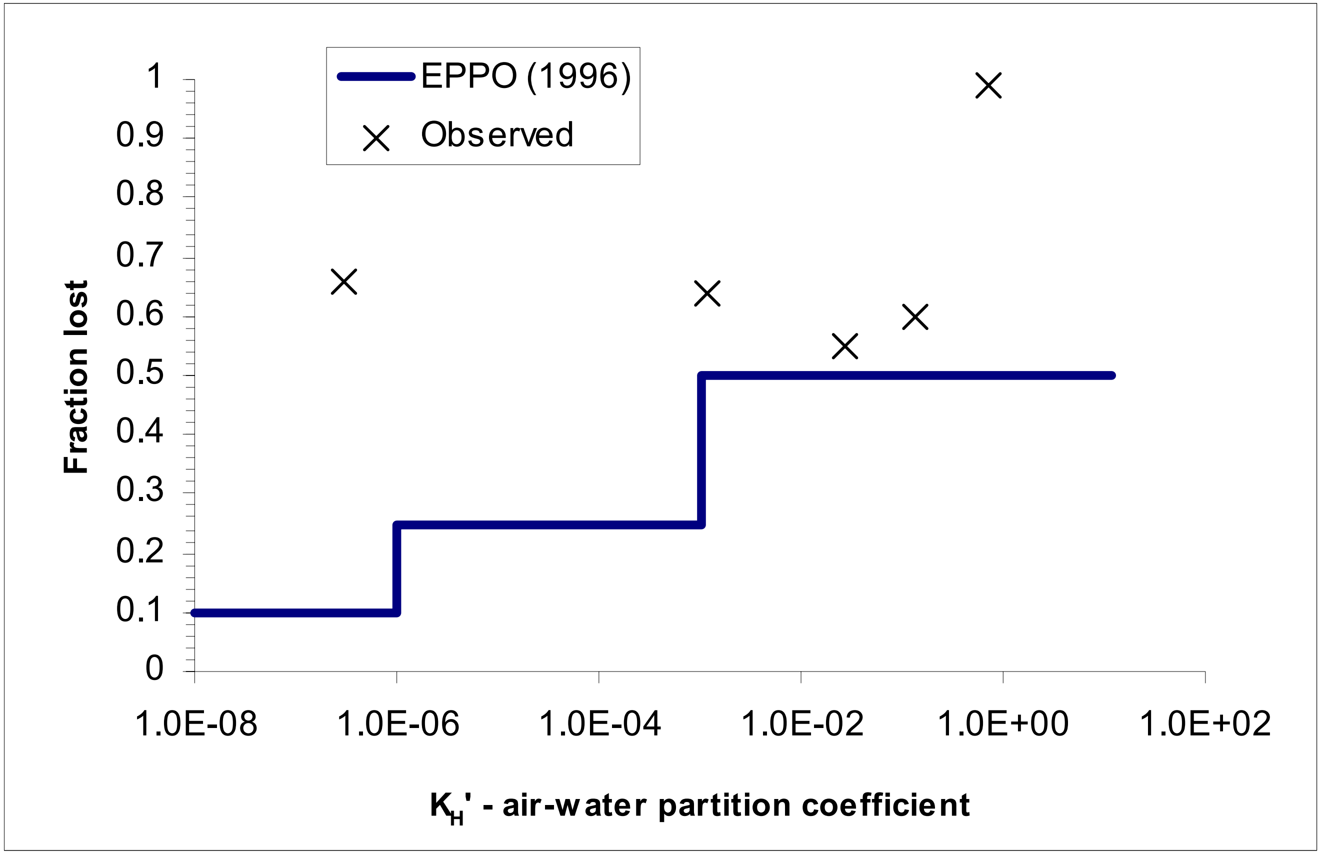
Daily loss fraction by evaporation from leaves



European and Mediterranean Plant Protection Organisation (EPPO), *Council of Europe, 96/5543*

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Degradation on leaves

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Photolysis rate constants rarely available

Degradation on leaves modelled as photocehmical oxidation, i.e. based on k_{OH} and assumed OH concentration in troposphere above field

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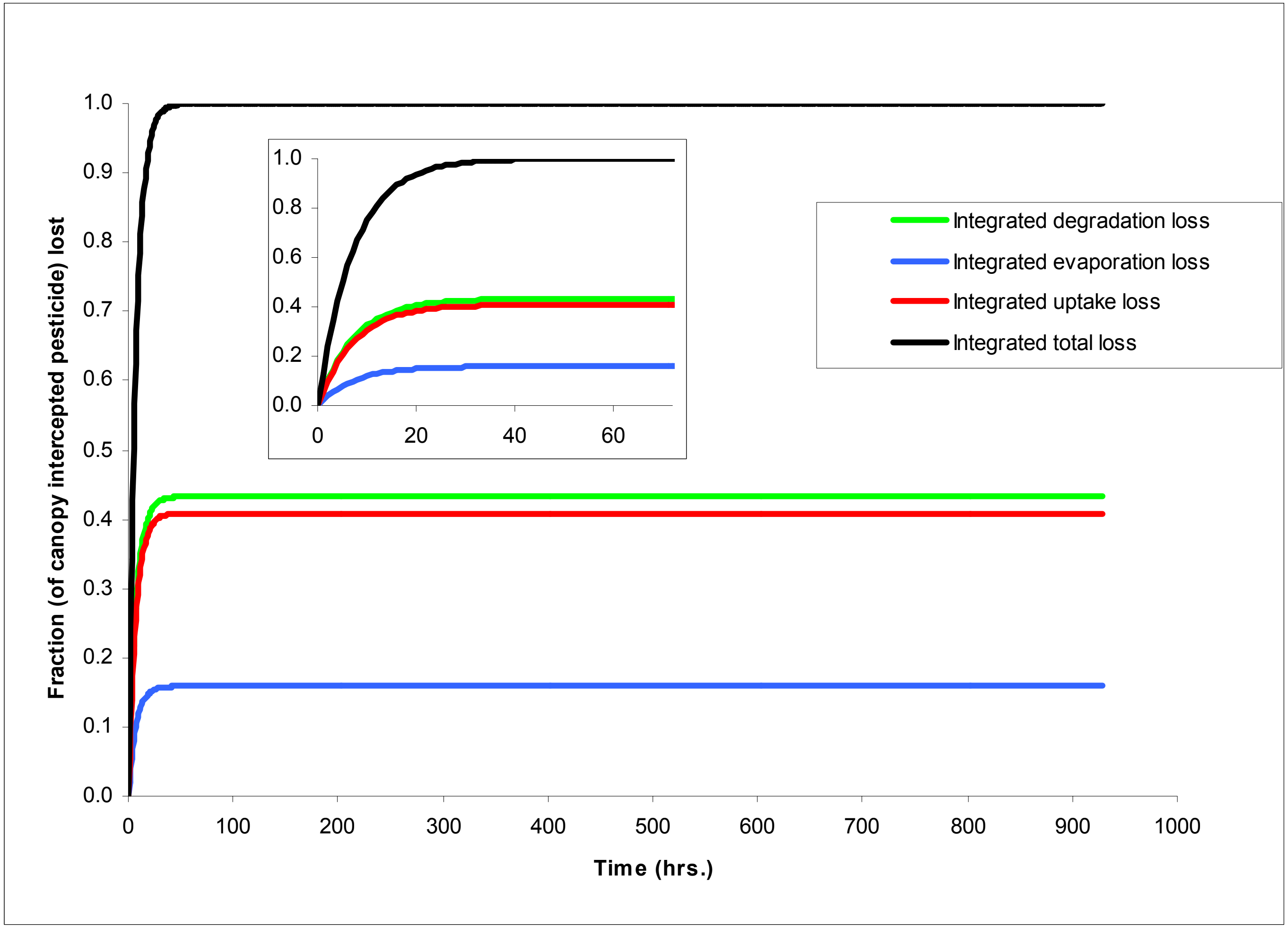
Combined leaf fate of α-cypermethrin

Uptake, evaporation and degradation of α-cypermethrin

(log K_{ow}=6.9, $T_{½,air}$=0.5d, MV=313cm^3/mol)



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Degradation and evaporation from surface soil

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- Competing processes occurring between application and next precipitation event
- After precipitation event, run-off and leaching are the only soil processes modelled
- Degradation modelled as first order process from $t_{½,soil}$ - corrected for temperature dependence
- Evaporation modelled as diffusion over boundary layer above soil assuming zero air concentration

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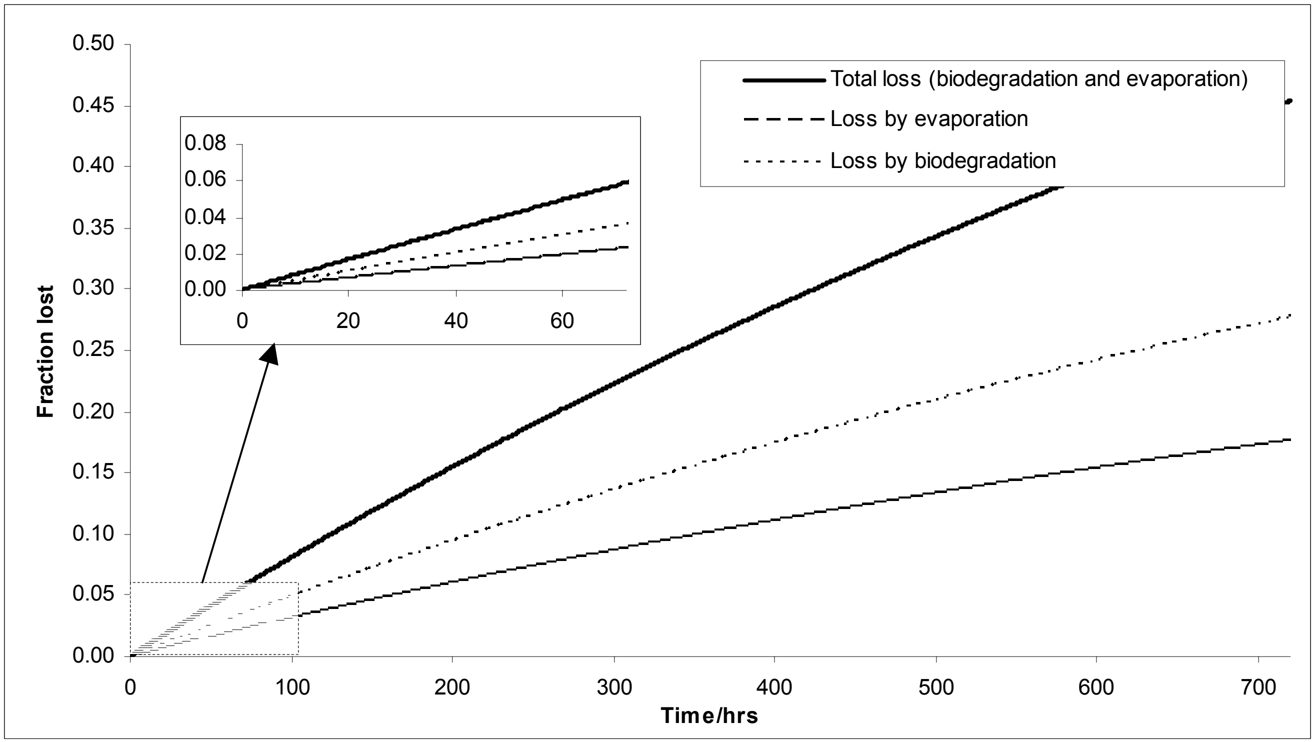
Degradation and evaporation from surface soil

Combination of soil evaporation and biodegradation in top soil for Alclonifen (vapour pressure = 1.20×10^{-7} mm Hg, $t_{1/2}$ = 40 days, temp. 20 ºC)



Default duration from application to precipitation 3 days

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Run-off and leaching

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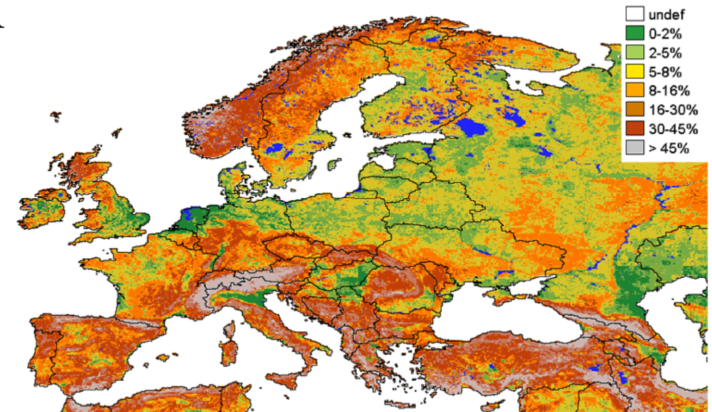
Surface run-off determined from

- Sand content of soil
- Slope of field
- Annual excess rain



Leaching determined from adsorption and degradation between 1 and 60 cm soil depth

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Drainage divides leachate between surface waters and groundwater

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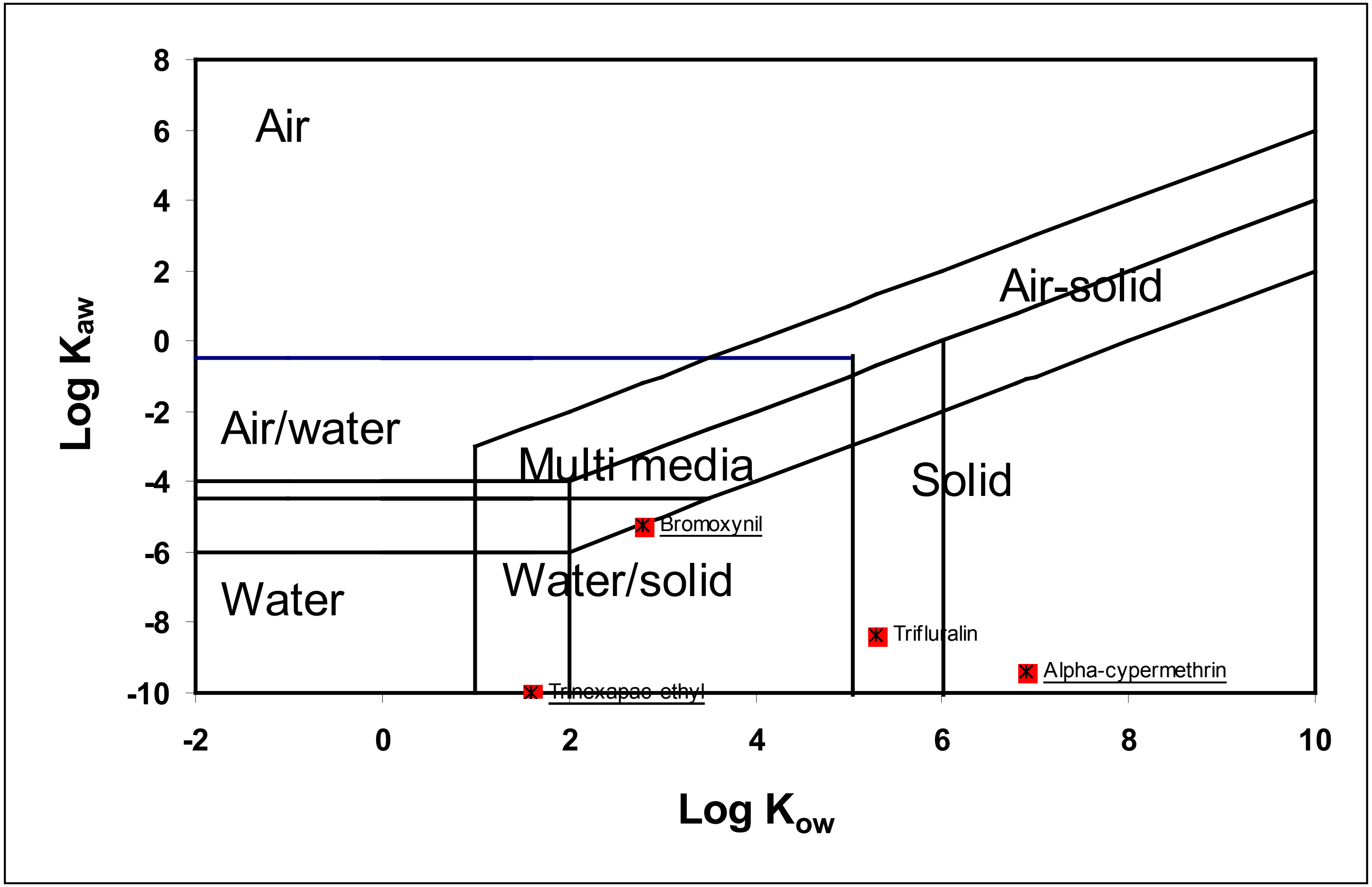
$$f_{gw} = f_{l,i}(1-\delta)$$

In Denmark, the frequency of drainage is $\delta=0.55$

The results

Examples for four different combination of pesticides and application type:



M.Margni, D.Pennington, M. Birkved, H.F. Larsen & M. Hauschild: Test set of organic chemicals for LCIA characterisation method comparison - Contribution to Work-package 7 of the OMNIITOX Project.

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Properties of selected pesticides

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Name	**Type**	**Log K_{ow}**	**Log K_{aw}**	**Soil $t_{½}$ (days)**	**Air $t_{½}$ (days)**
Bromoxynil	Herbicide	2.8	-5.2	2.4	51
Trinexapac-ethyl	Growth regulator	1.6	-10	0.22	0.1
Trifluralin	Herbicide	5.3	-8.3	83	0.5
Alpha-cypermethrin	Insecticide	6.8	-9.4	8.0	0.4

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Application of pesticides

Name	Crop	Development stage	Month
Trinexapac-ethyl	Cereals	I	May
Bromoxynil	Cereals	II	June
Alpha-Cypermethrin	Cereals	IV	August
Trifluralin	Cabbage	II	June

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Primary distribution

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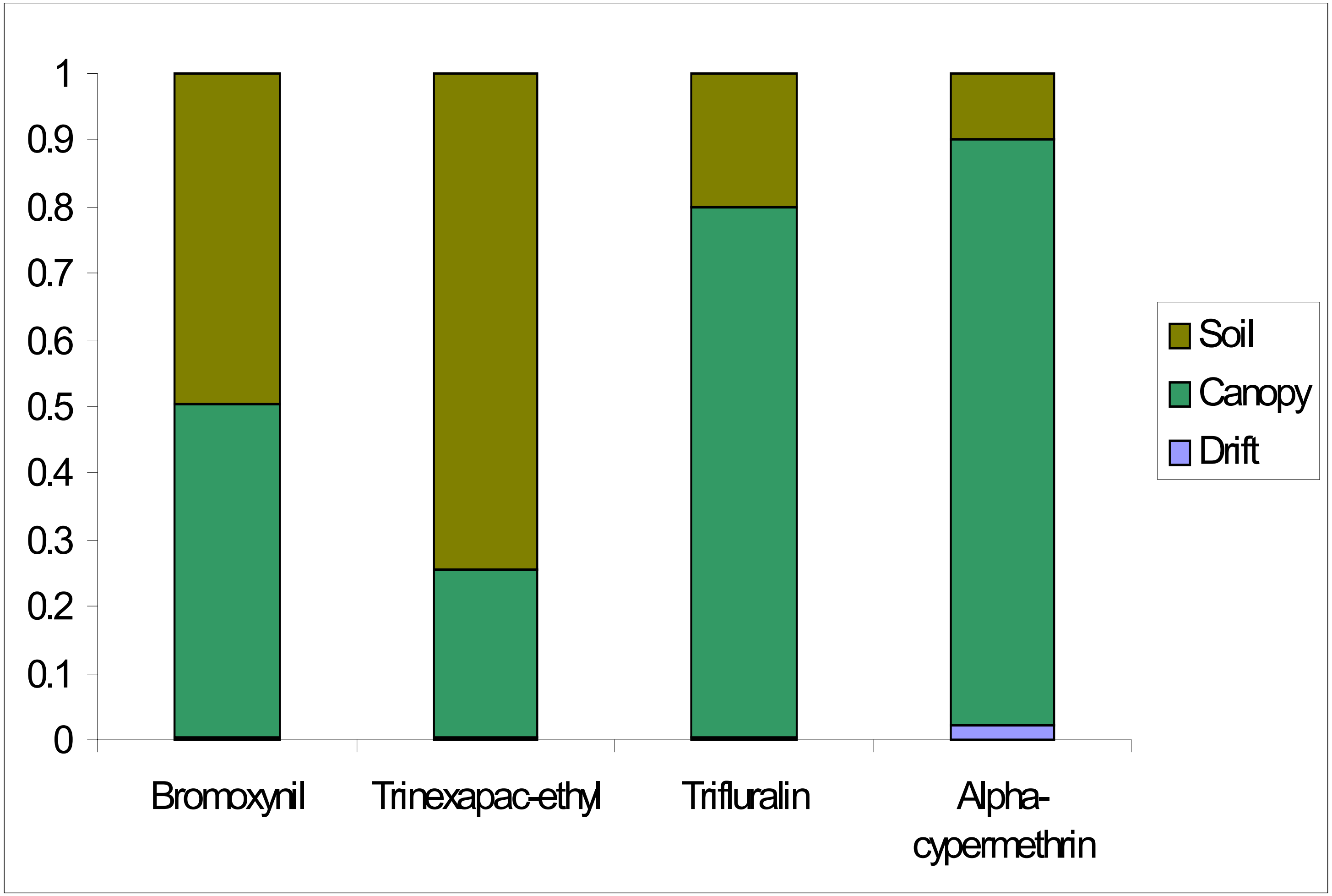

Name	Crop	Development stage	Month
Trinexapac-ethyl	Cereals	I	May
Bromoxynil	Cereals	II	June
Alpha-Cypermethrin	Cereals	IV	August
Trifluralin	Cabbage	II	June

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Secondary distribution from leaves

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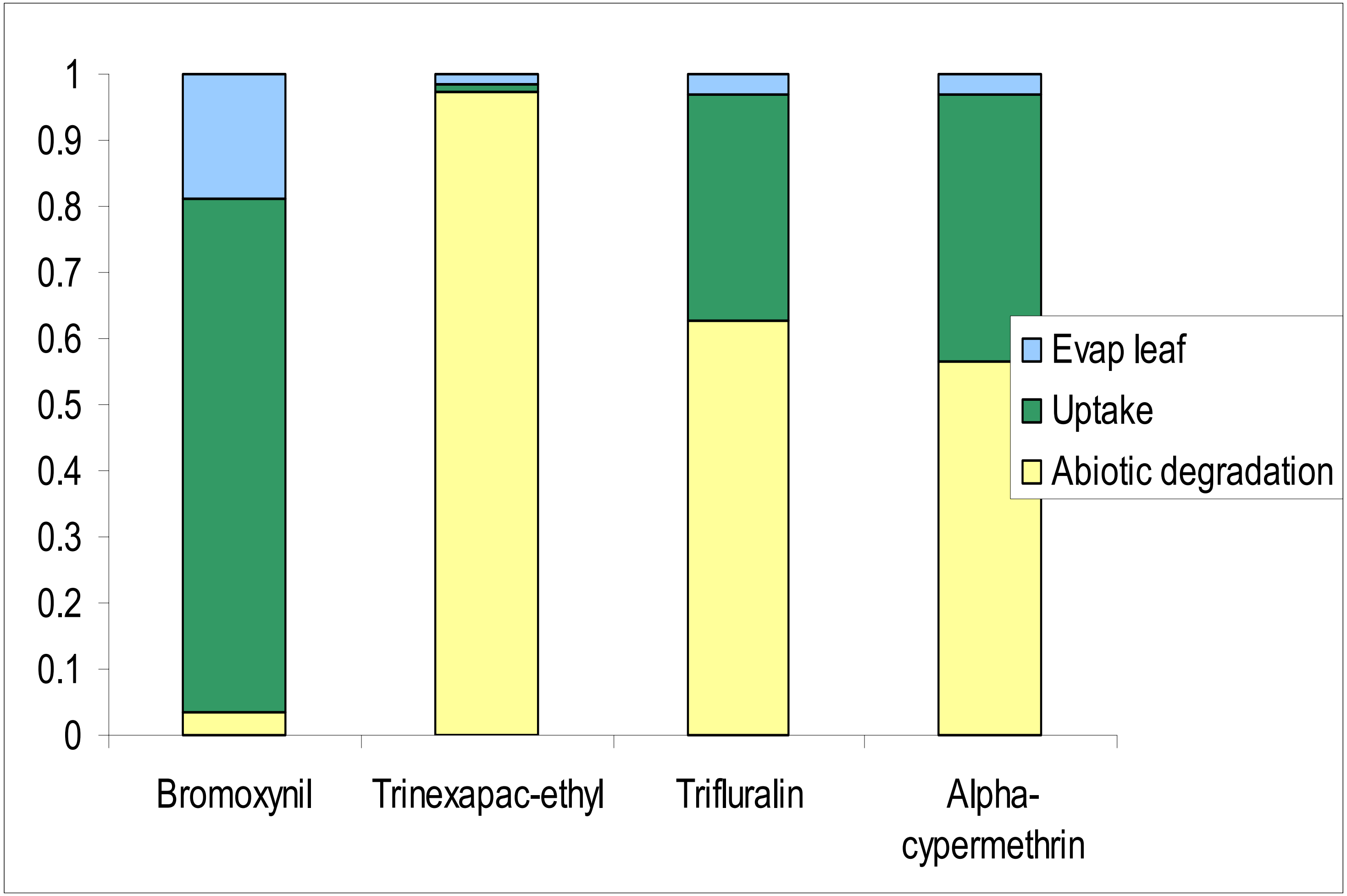

Name	Log K_{ow}	Log K_{aw}	Air $t_{½}$ (days)
Bromoxynil	2.8	-5.2	51
Trinexapac-ethyl	1.6	-10	0.1
Trifluralin	5.3	-8.3	0.5
Alpha-cypermethrin	6.8	-9.4	0.4

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Secondary distribution from soil

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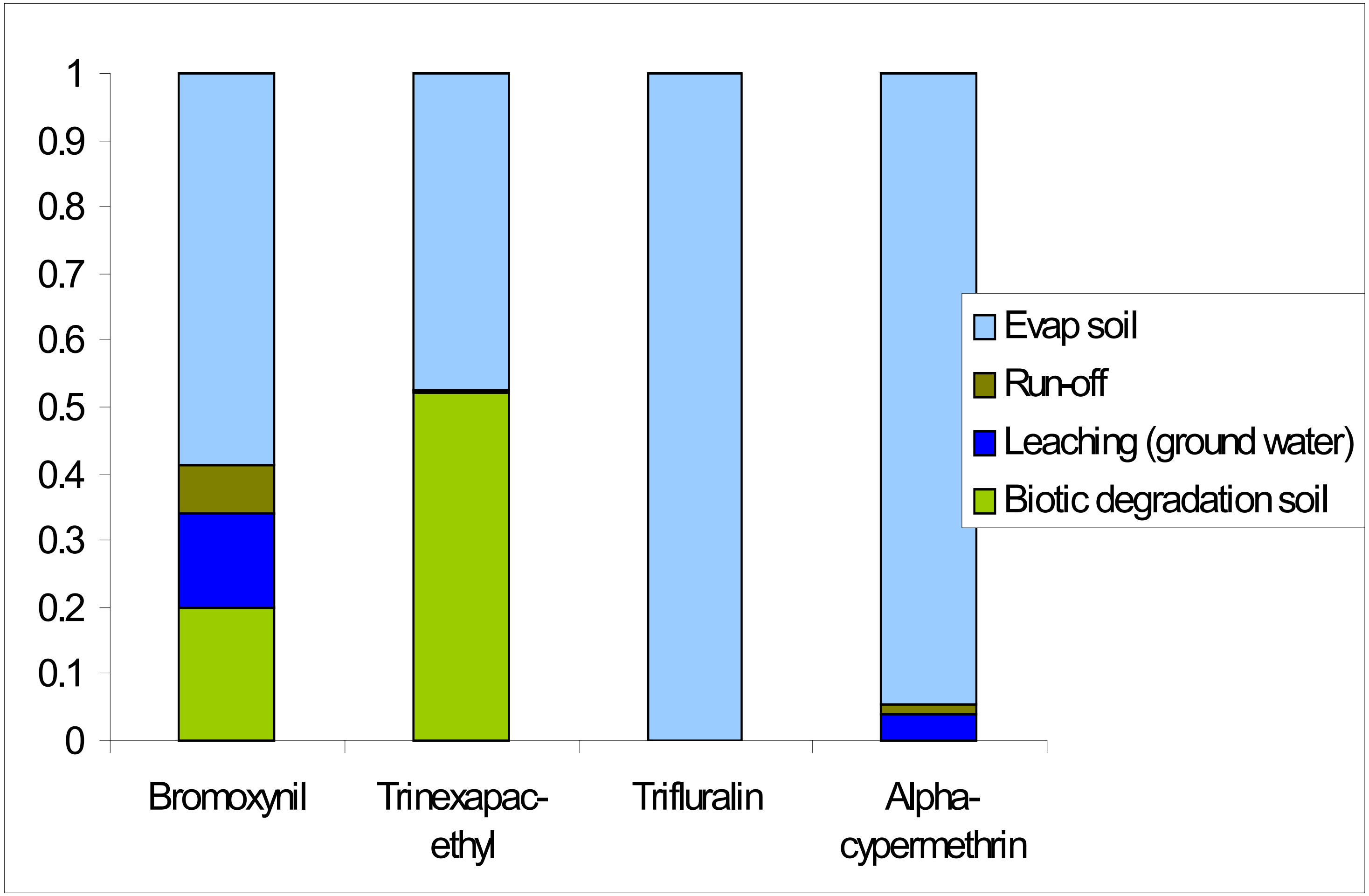

Name	Log K_{ow}	Log K_{aw}	Soil $t_{½}$ (days)
Bromoxynil	2.8	-5.2	2.4
Trinexapac-ethyl	1.6	-10	0.22
Trifluralin	5.3	-8.3	83
Alpha-cypermethrin	6.8	-9.4	8.0

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Overall distribution pattern

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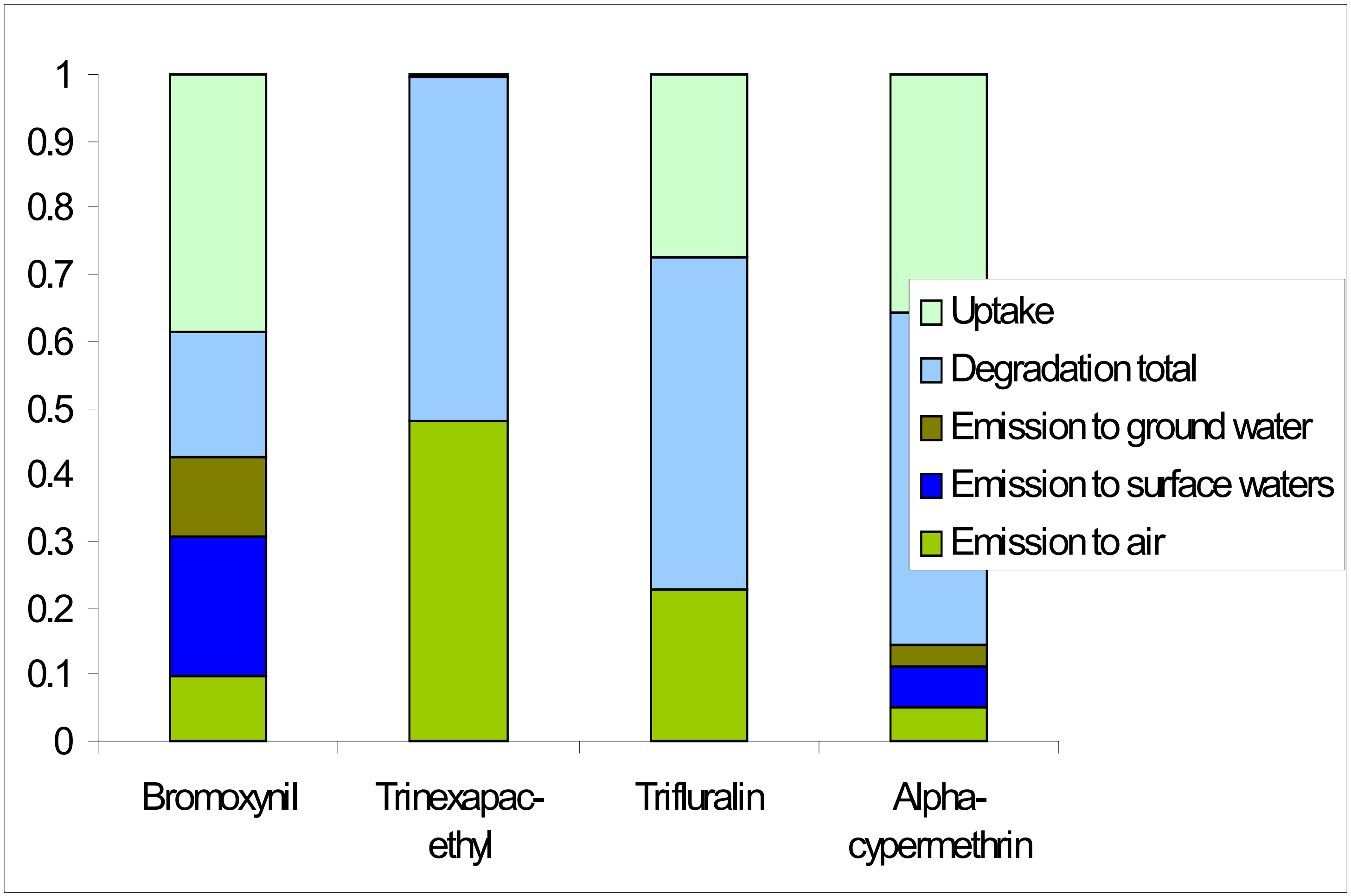

Name	Log K_{ow}	Log K_{aw}	Soil $t_{½}$ (days)	Air $t_{½}$ (days)
Bromoxynil	2.8	-5.2	2.4	51
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Overall distribution pattern

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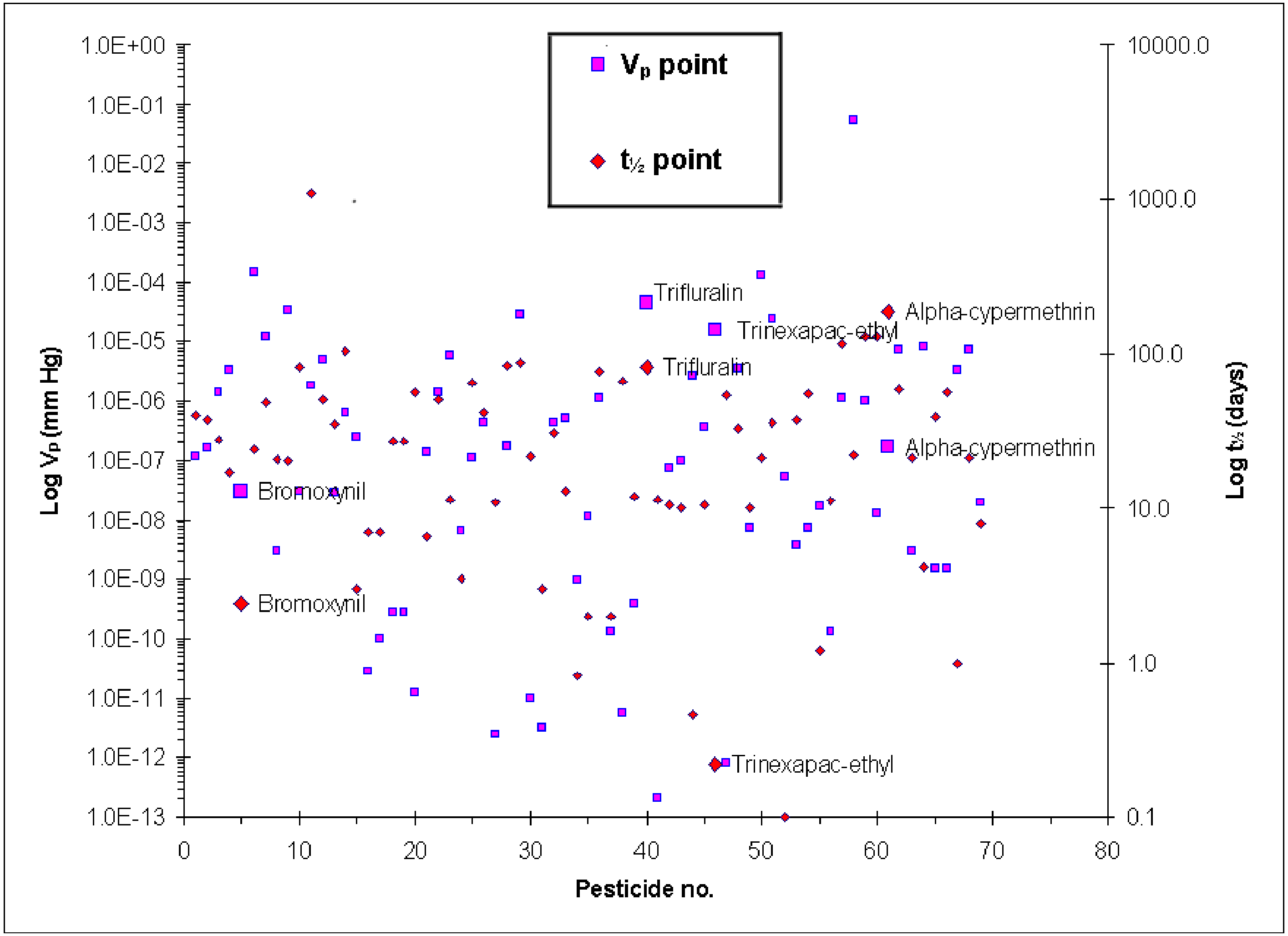

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The results

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Emission to air

- Drift + evaporation from plant + evaporation from soil

$$f_{air} = f_w + f_p \times f_{vp} + f_s \times f_{vs}$$

Emission to water

- Drained leachate + surface run-off

$$f_{water} = (f_r + f_d) \times f_s$$

Emission to groundwater

$$f_{groundwater} = (1 - \delta) \times f_d \times f_s$$

Emission to soil

$$f_{soil} = 0$$

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The results

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Output: Inventory results

All figures in kg per functional unit

Name	Type	Applied quantity	Emission to			
			Air	Water	Groundwater	Soil
Bromoxynil	Herbicide	3.83	0.38	0.80	0.45	0
Trinexapac-ethyl	Growth regulator	1.33	0.64	0.00011	0.00007	0
Trifluralin	Herbicide	8.3	1.88	0.0070	0.0035	0
Alpha-cypermethrin	Insecticide	0.6	0.031	0.036	0.021	0

Input: Pesticide and management parameters

Pesticide data: molecular weight, molecular volume, solubility, vapour pressure, pK_a, $LogK_{ow}$, K_{oc}, K_H, $t_{½,soil}$, k_{OH}

Application type, crop type and development stage – rest by default

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The further work

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Further testing of the model in the Danish project: LCA of Basic Foods (Ministry of Agriculture)

Spatial differentiation of the model through adaptation to conditions in other countries

Compilation of national data for

- Slope factors
- Meteorological data (precipitation, temperature, wind speed, …)
- Pedological data (soil texture)
- Other crop types?
- ….

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The references

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Within one week available for download from: http://ipt.dtu.dk/~mic/

Birkved, M. and Hauschild, M.: PESTLCI – a Pesticide distribution model for LCA -Development of a Pesticide distribution model for use in life cycle inventory analysis. IPL-DTU, 2003

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EDIP97 characterisation factors for all 69 pesticides allowed for use on field crops in Denmark

PESTLCI Excel spreadsheet model available on request from mob@ipl.dtu.dk