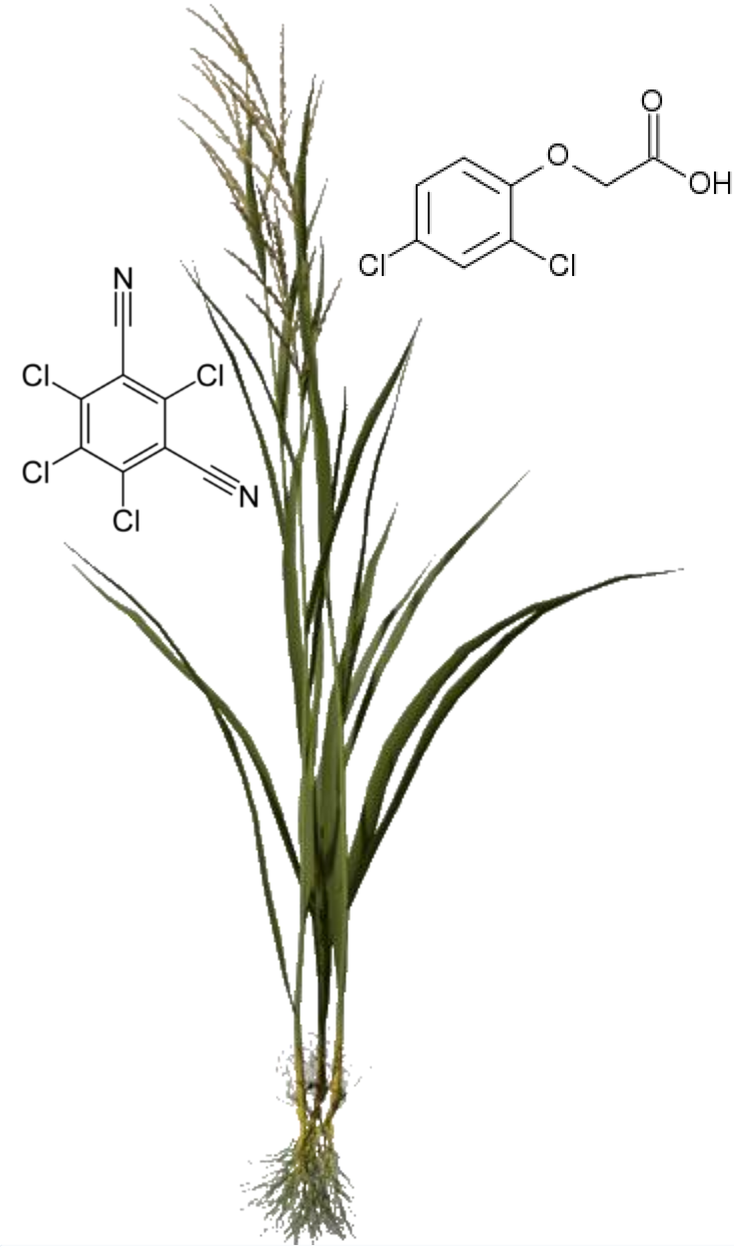


Dynamic multi-crop model to characterize impacts of pesticides in food

P. Fantke, R. Juraske

A. Antón, E. Sevigné, A. Kounina

Which food crop has highest pesticide load?

Goals

After the course, all participants will be able to:

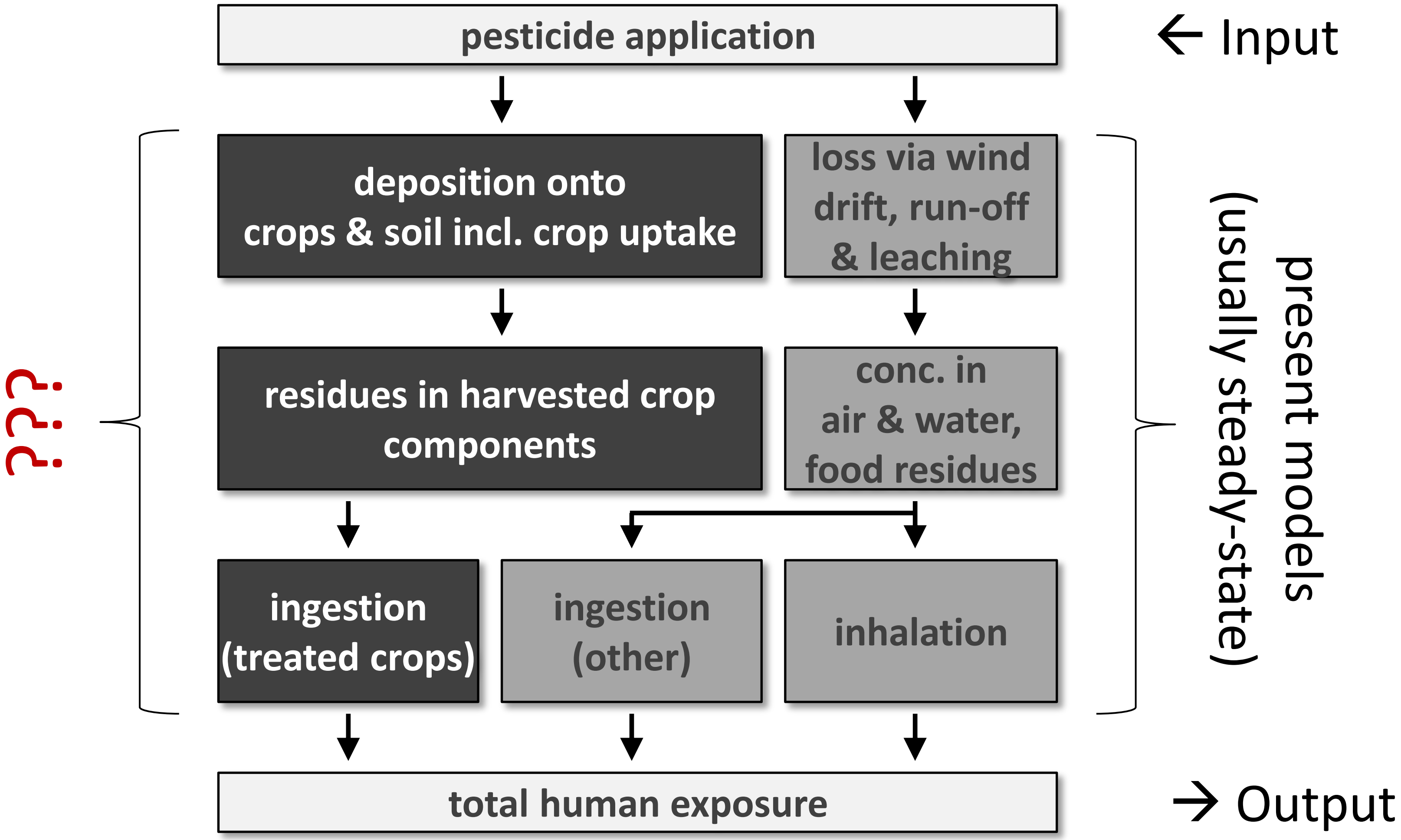
- Explain the principles and processes involved in the distribution of pesticides applied to different food crops,
- Quantify potential health impacts from pesticide intake via food crop consumption, and
- Discuss different potentials for pesticide substitution.

Contents

- Background and scope
- Mass balance system
- From harvest fraction to intake fraction
- Characterization: factors and model
- Pesticide substitution
- Highlights and Summary

- **Background and scope**
- Mass balance system
- From harvest fraction to intake fraction
- Characterization: factors and model
- Pesticide substitution
- Highlights and Summary

Problem Statement



pesticide application

← Input

deposition onto crops & soil incl. crop uptake

loss via wind drift, run-off & leaching

residues in harvested crop components

conc. in air & water, food residues

ingestion (treated crops)

ingestion (other)

inhalation

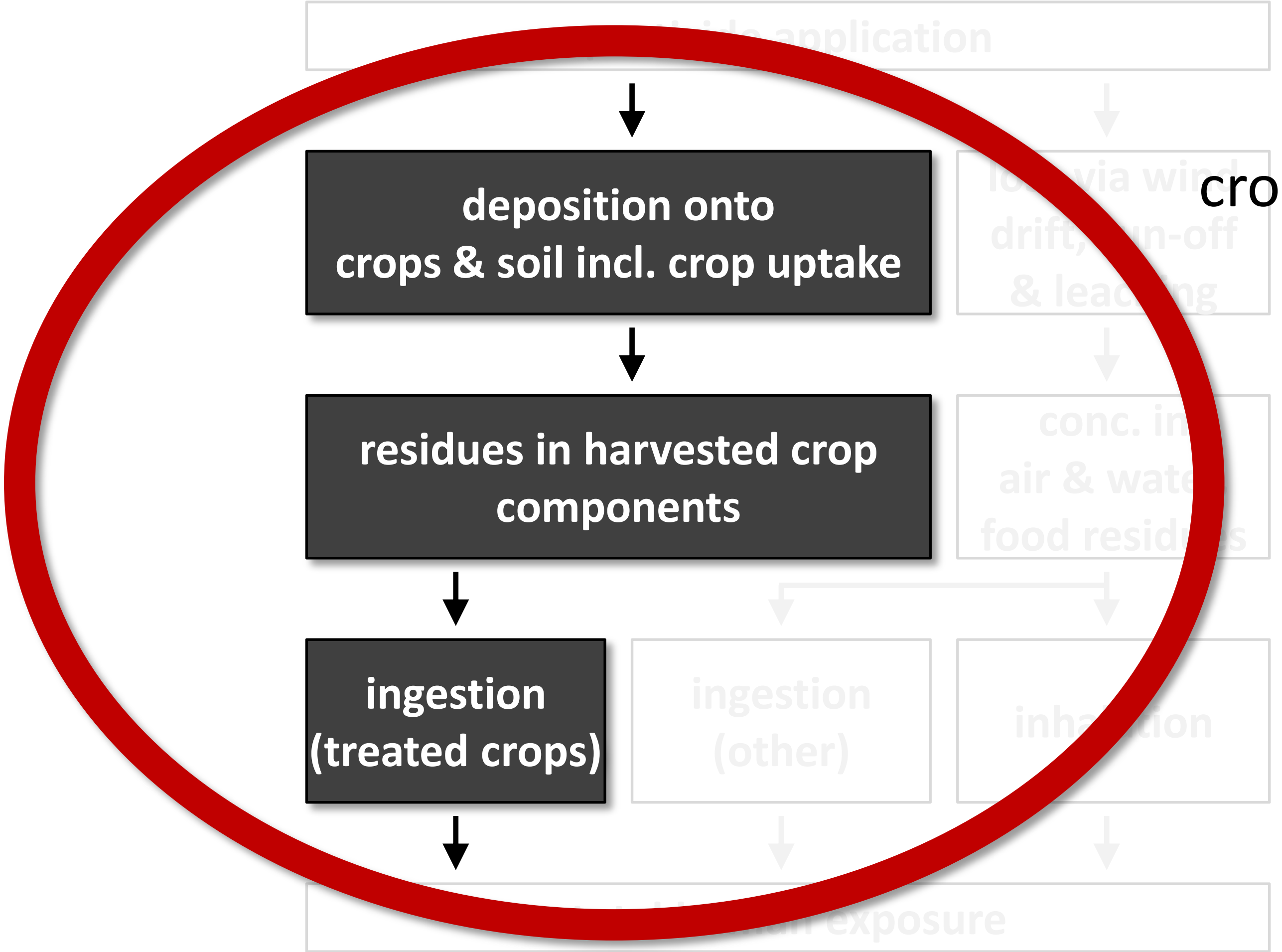
total human exposure

→ Output

???

present models (usually steady-state)

Problem Statement


deposition onto crops & soil incl. crop uptake

residues in harvested crop components

ingestion (treated crops)

Problem:
crop residues so far
not considered!

Followed Approach – Aim

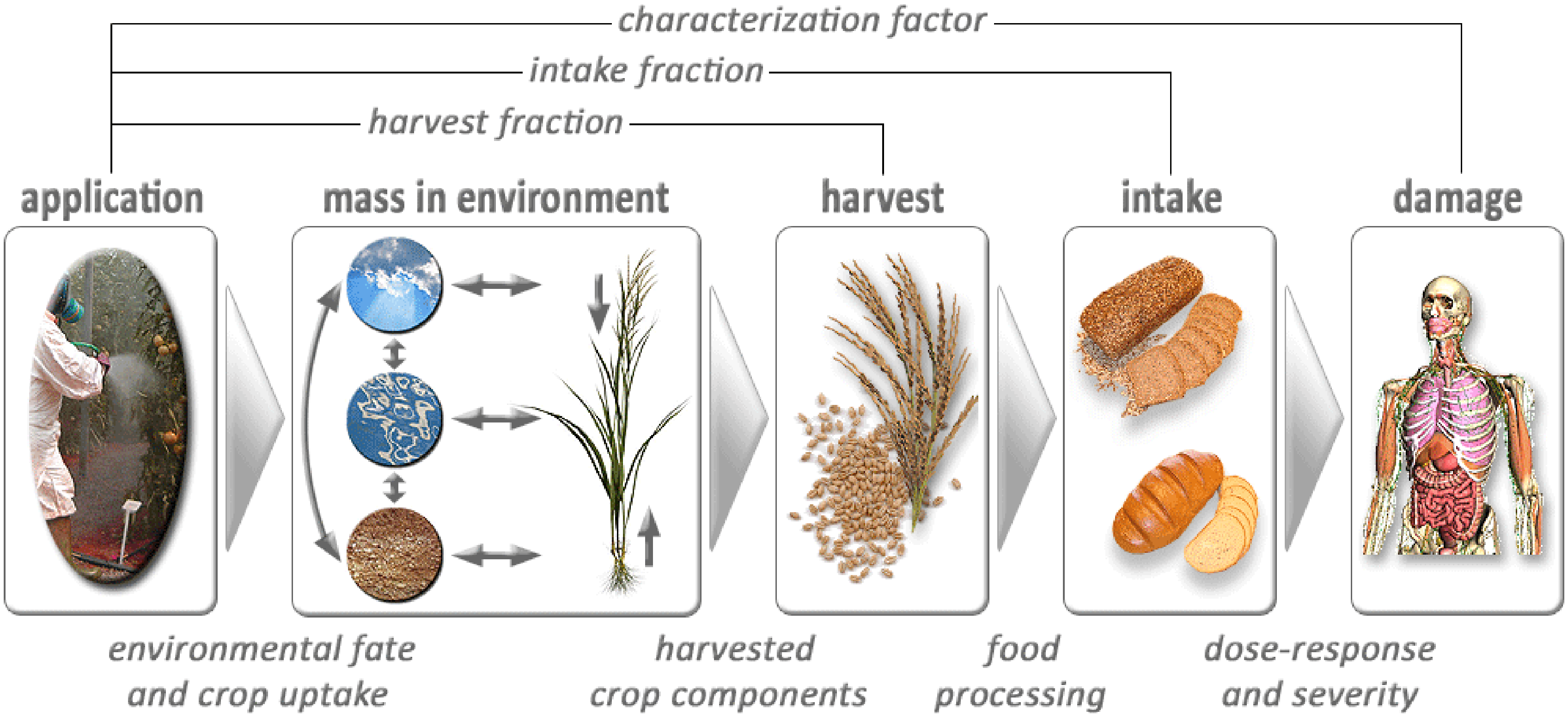
We aim at …

- Quantifying potential health impacts caused by pesticide use (no arbitrary measures like ‘MRL’),
- Comparing pesticides in terms of their health impact,
- Giving recommendations for optimizing pesticide use.

Methodological tool of choice …

- Life Cycle Impact Assessment (LCIA)
- Based on average values, not worst case assumptions (basis for comparative assessment)

Followed Approach – Impact Pathway



Followed Approach – Scope

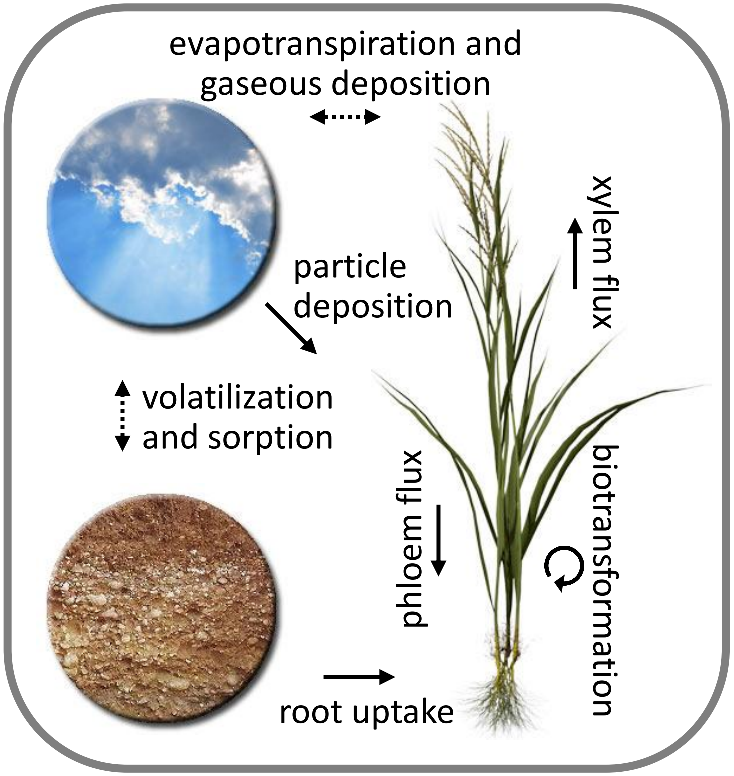
Considered crops:

Wheat	(68% of cereals)
Paddy rice	(97% of paddy cereals)
Tomato	(15% of herbaceous vegetables)
Apple	(13% of fruit trees)
Lettuce	(14% of leafy vegetables)
Potato	(51% of roots and tubers)

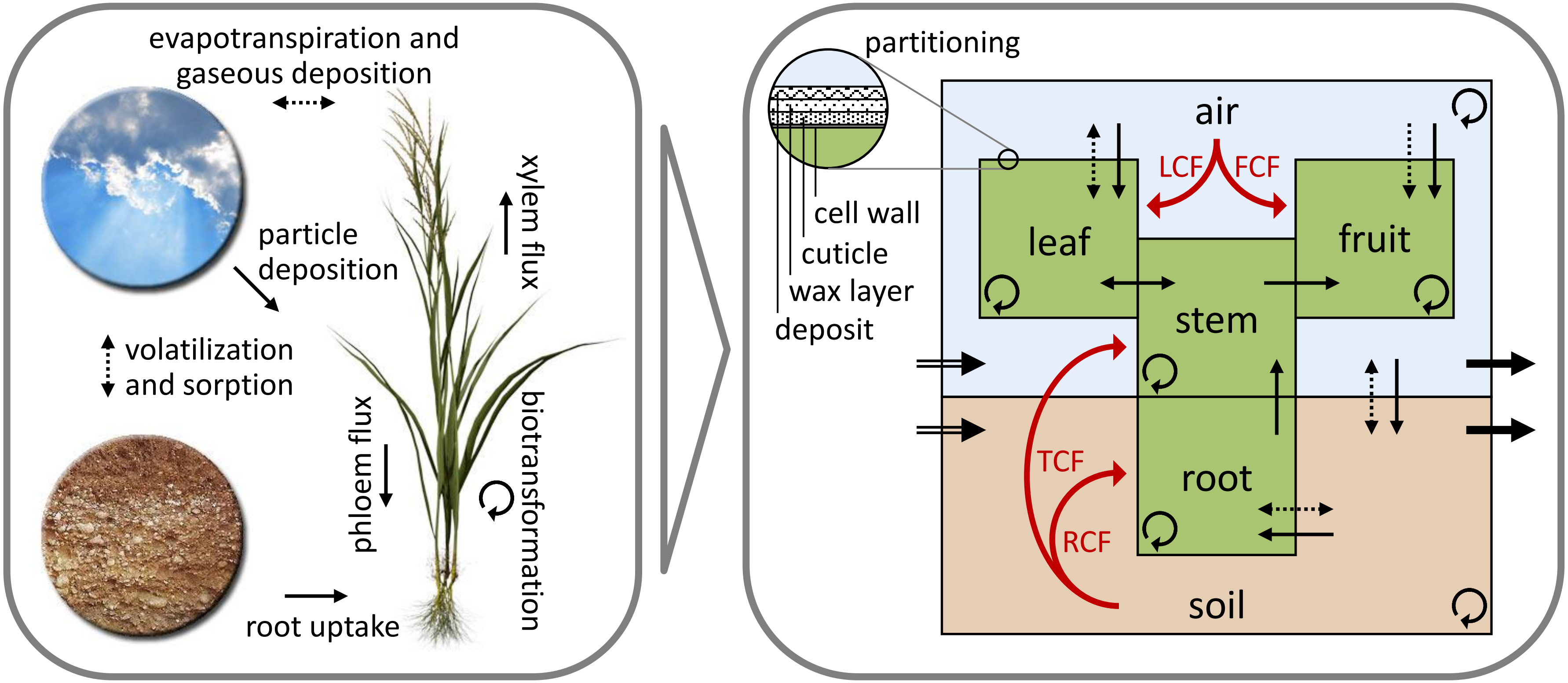
$\underbrace{\qquad\qquad\qquad\qquad\qquad\qquad}_{\text{45\% of global vegetal consumption}}$

- Background and scope
- **Mass balance system**
- From harvest fraction to intake fraction
- Characterization: factors and model
- Pesticide substitution
- Highlights and Summary

Physical System



Modeled System



⇒ system input
➡ system loss
⋯▸ diffusive transfer
→ advective transfer
↻ degradation

Modeled System – Mass Balance

$$\frac{\mathrm{d}\vec{m}(t)}{\mathrm{d}t} = \mathbf{K}\,\vec{m}(t)$$

$\vec{m}$: vector of masses [kg]
$\mathbf{K}$: matrix of rate constants k [d^{-1}]
t : time [d]

Solution for pulse application …

$$\vec{m}(t) = \exp(\mathbf{K}\,t)\;\vec{m}(0)$$

→ System will be diagonalized (decomposed) to arrive at solution with matrix exponential

→ Further reading: Fantke et al., 2013, *EMS*, 40: 316-324

Mass Balance – Rate Constants

$$\frac{\mathrm{d}\vec{m}(t)}{\mathrm{d}t} = \mathbf{K}\,\vec{m}(t)$$

$\vec{m}$: vector of masses [kg]
K : matrix of rate constants k [d^{-1}]
t : time [d]

↓

Matrix of rate constants for …

- Diffusive/advective transfers between compartments
  → ‚off-diagonal elements‘
- Degradation processes within compartments
  → incorporated into ‚main diagonal elements‘

Mass Balance – Rate Constants

$$\frac{\mathrm{d}\vec{m}(t)}{\mathrm{d}t} = \mathbf{K}\,\vec{m}(t)$$

$\vec{m}$: vector of masses [kg]

$\mathbf{K}$: matrix of rate constants k [d^{-1}]

t : time [d]

$$\mathbf{K} := \begin{array}{c|cccc} & \text{air} & \text{soil} & \cdots & \text{leaf} \\ \hline \text{air} & -k_{\text{air,total}} & k_{\text{air}\leftarrow\text{soil}} & \cdots & k_{\text{air}\leftarrow\text{leaf}} \\ \text{soil} & k_{\text{soil}\leftarrow\text{air}} & -k_{\text{soil,total}} & & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ \text{leaf} & k_{\text{leaf}\leftarrow\text{air}} & 0 & \cdots & -k_{\text{leaf,total}} \end{array}$$

Mass Balance – Rate Constants

$$\frac{\mathrm{d}\vec{m}(t)}{\mathrm{d}t} = \mathbf{K}\,\vec{m}(t)$$

$\vec{m}$: vector of masses [kg]
K : matrix of rate constants k [d^{-1}]
t : time [d]

$$\downarrow$$

$$\mathbf{K} = \begin{pmatrix} k_{11} & \cdots & k_{1n} \\ \vdots & \ddots & \vdots \\ k_{n1} & \cdots & k_{nn} \end{pmatrix} \text{ with } k_{ij} = \begin{cases} k_{ij} & \text{for } i \neq j \\ -\left(k_{\mathrm{loss},i} + \sum\limits_{l=1,\, l\neq i}^{n} k_{li}\right) & \text{for } i = j \end{cases}$$

Mass Balance – Initial Conditions

$$\frac{\mathrm{d}\vec{m}(t)}{\mathrm{d}t} = \mathbf{K}\,\vec{m}(t)$$

↓

$\vec{m}$: vector of masses [kg]

$\mathbf{K}$: matrix of rate constants k [d^{-1}]

t : time [d]

Initial mass (applied pesticide mass) …

- Is defined as part of vector $\vec{m}(t)$ at time $t = 0$

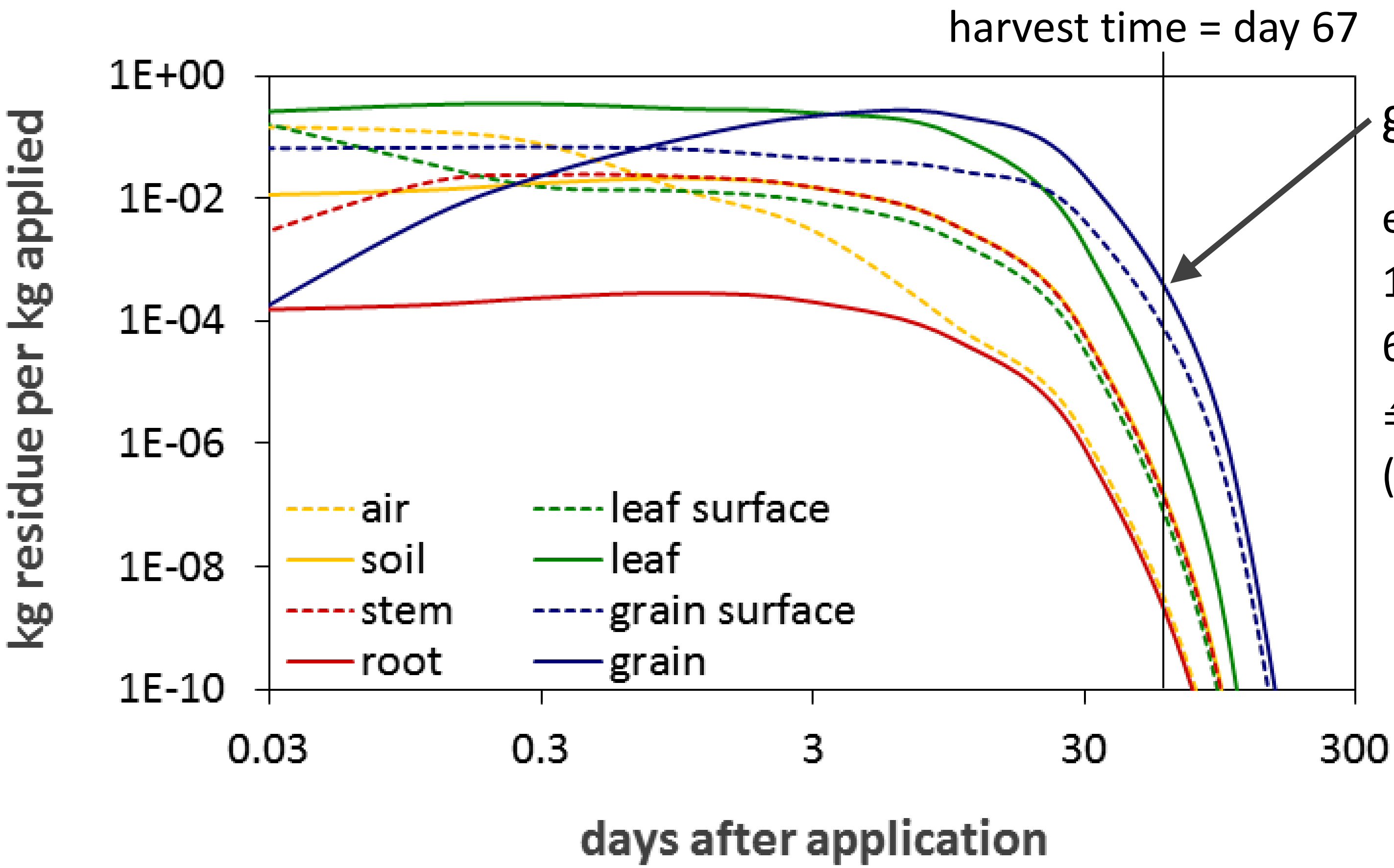
  → application time

Final mass (pesticide residues) …

- Vector $\vec{m}(t)$ at time $t > 0$ → harvest time

Mass Balance – Example

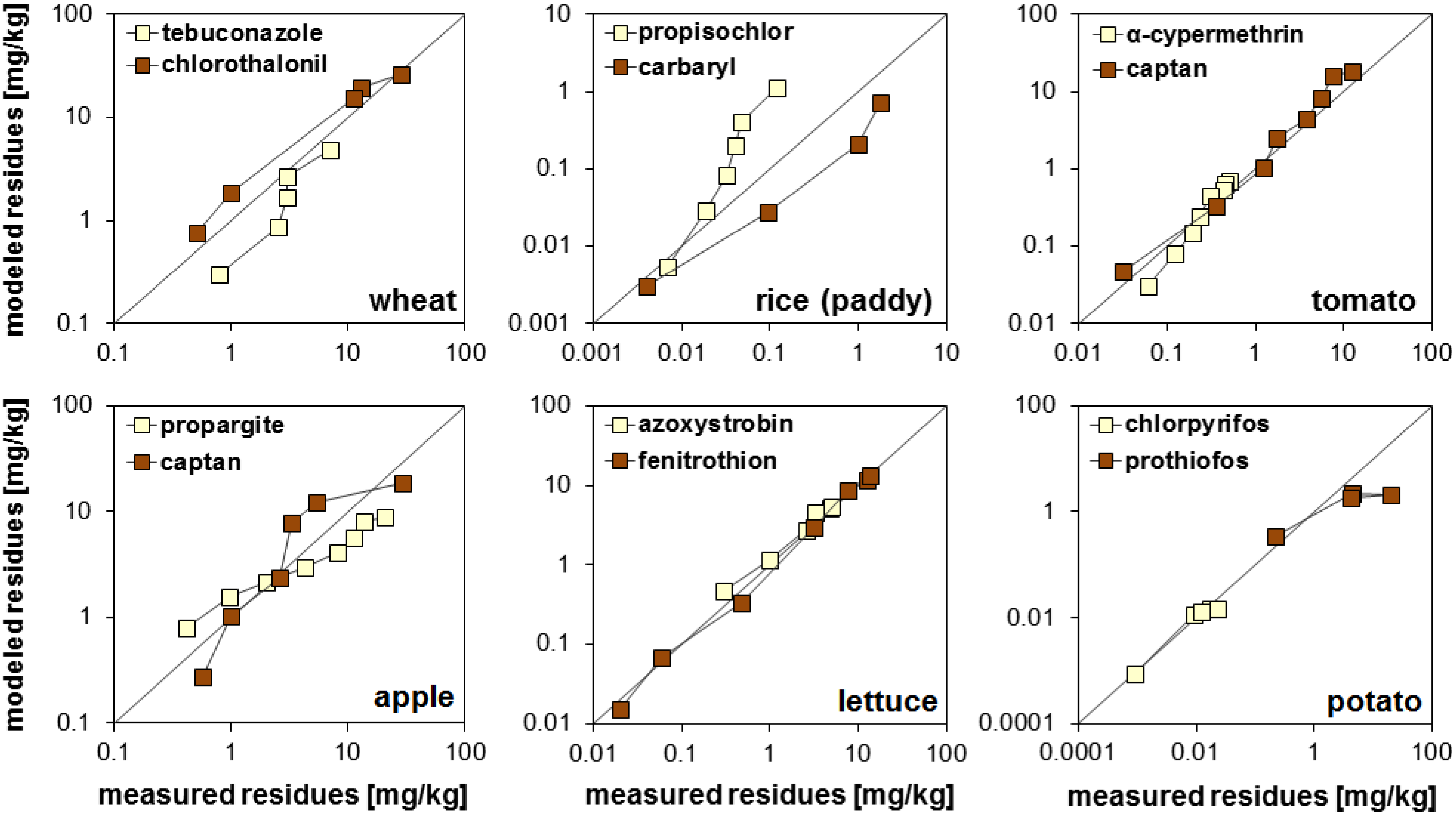
Insecticide cyromazine applied to wheat



grains: 0.28 g/kg

example:
100 g applied/ha,
6 t grain yield/ha
≙ 4.7 µg/kg_{grains}
(MRL: 50 µg/kg_{grains})

Mass Balance – Evaluation



- Background and scope
- Mass balance system
- **From harvest fraction to intake fraction**
- Characterization: factors and model
- Pesticide substitution
- Highlights and Summary

Harvest Fraction

Mass in all harvested crop parts relative to total applied mass

$$hF = \frac{\sum_{i=1}^{n} m_i(t)}{m_{\mathrm{app}}}$$

→ Pesticide mass in harvest

→ Applied pesticide mass

hF : harvest fraction [$\mathrm{kg_{in\ harvest}/kg_{applied}}$]
m_i : residual mass in compartment i [$\mathrm{kg_{in\ harvest}}$]
m_{app} : total applied mass [$\mathrm{kg_{applied}}$]
t : harvest time [d]

Intake Fraction

Mass taken in via consumption relative to total applied mass

$$iF = hF \times PF$$

↓

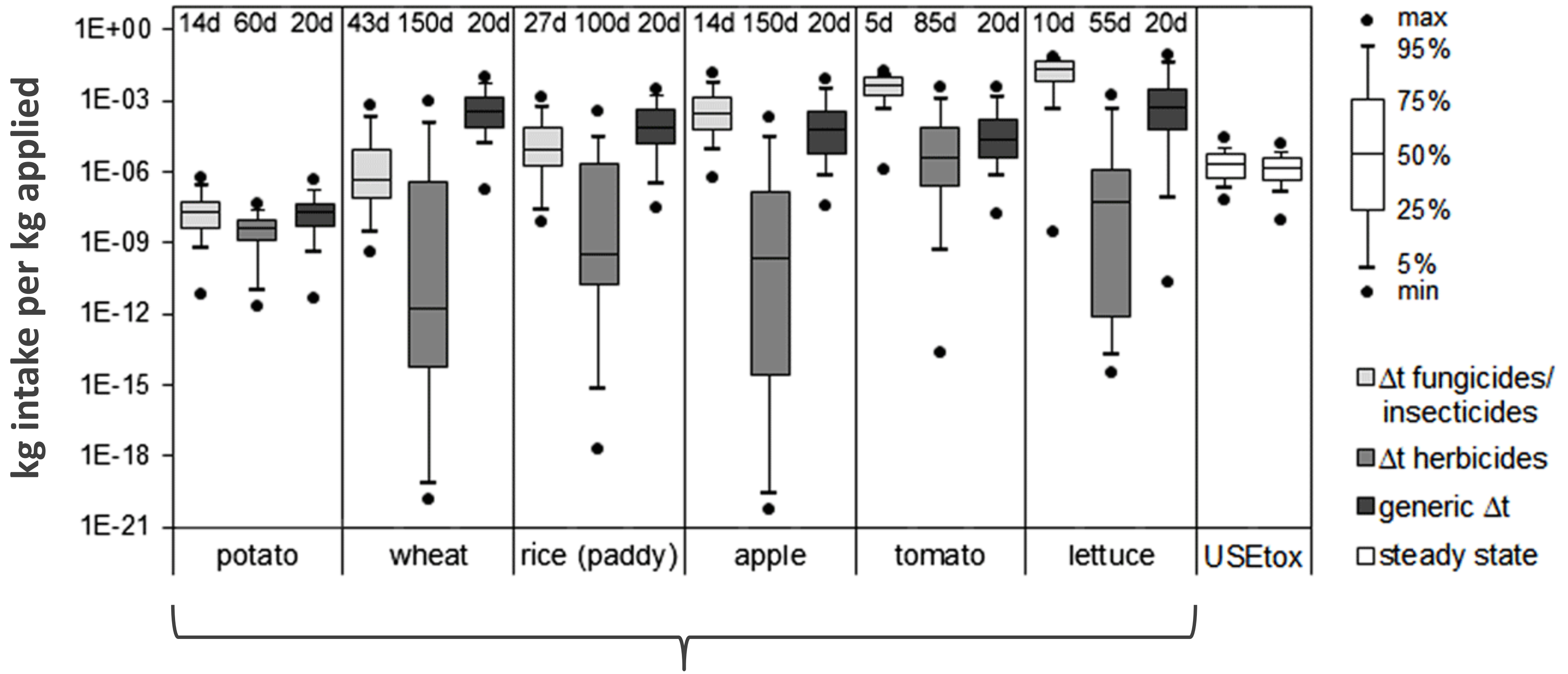
iF : human intake fraction [$\mathrm{kg_{intake}/kg_{applied}}$]
hF : harvest fraction [$\mathrm{kg_{in\ harvest}/kg_{applied}}$]
PF : food processing factor [$\mathrm{kg_{intake}/kg_{in\ harvest}}$]

Food processing …

Intake Fraction – Example

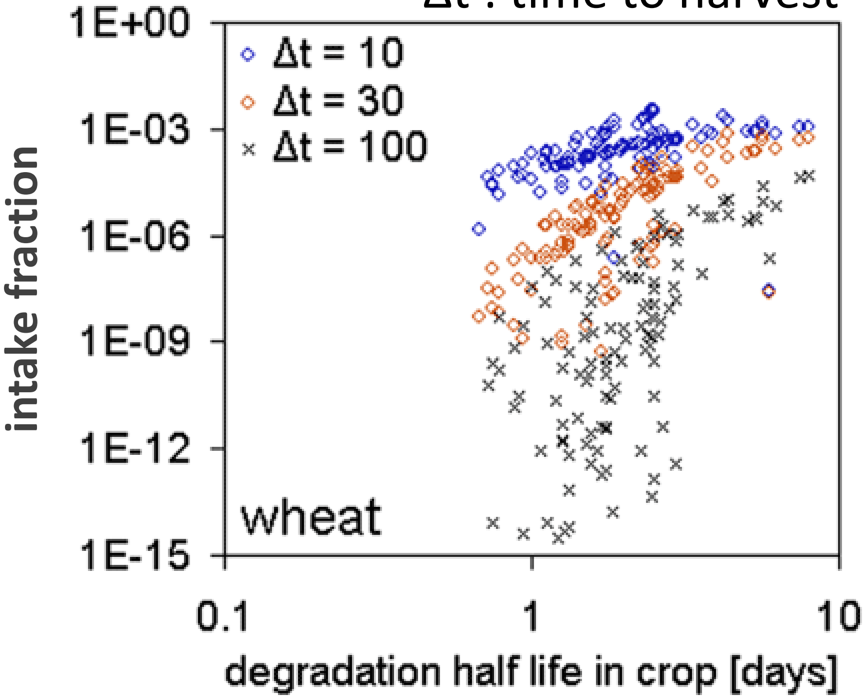
Comparison of 121 pesticides

time to harvest

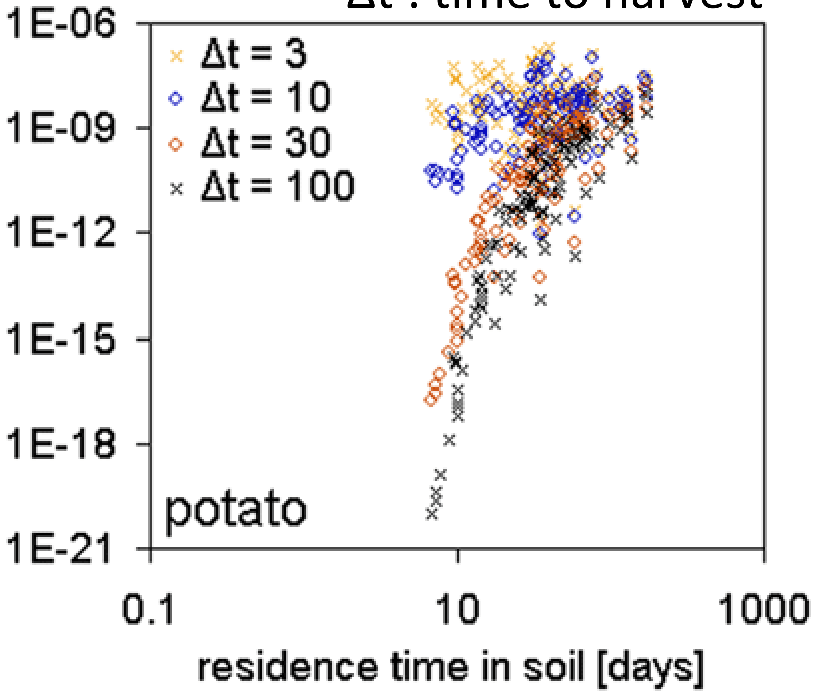


crop consumption

Intake Fraction – Influencing Aspects



Δt : time to harvest



Δt : time to harvest

- Background and scope
- Mass balance system
- From harvest fraction to intake fraction
- **Characterization: factors and model**
- Pesticide substitution
- Highlights and Summary

Characterization Factor

Human toxicity potential relative to total applied mass

$$CF = iF \times \underbrace{\beta \times DF}_{EF}$$

CF : human toxicity characterization factor [DALY/$\text{kg}_{\text{applied}}$]
iF : human intake fraction [$\text{kg}_{\text{intake}}$/$\text{kg}_{\text{applied}}$]
β : dose-response slope factor [incidence risk/$\text{kg}_{\text{intake}}$]
DF : severity factor [DALY/incidence]

$$\downarrow$$

Human toxicity effect factor [DALY/$\text{kg}_{\text{intake}}$]

→ DALY: disability-adjusted life year

Human Toxicity Effect Factor

Dose-response based on human trials → not available

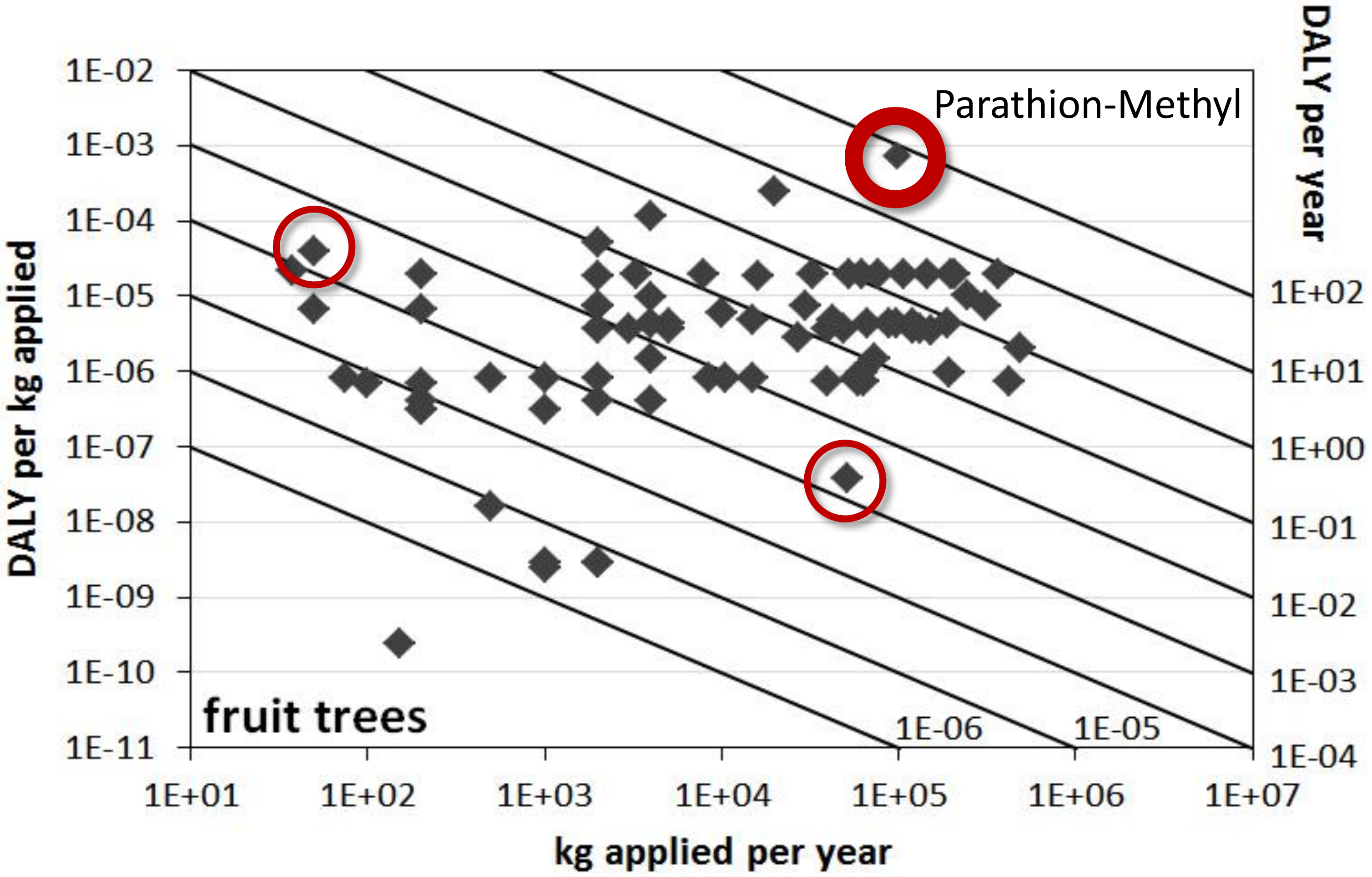
- Not ethically defendable
- Most human studies focus on acute exposure

Dose-response based on animal trials → uncertain!

- Cancer effects: derived from chronic lifetime dose affecting 50% of exposed population (ED_{50})
- Non-cancer effects: ED_{50} rarely available → ED_{50} estimated from no-observed effect level (NOEL) assuming linear slope

Characterization Factor – Application

Pesticides applied to fruit trees in EU24 in 2003



Characterization Model – dynamiCROP

dynamiCROP ...

- Is a dynamic plant uptake model,
- Covers human exposure to pesticides from crop intake,
- Includes various crop types,
- Is based on matrix algebra (flexible compartment set),
- Uses Matlab to solve the matrix exponential,
- Is available for download at **http://dynamicrop.org**

Characterization Model – Framework

dynamiCROP FRAMEWORK

INPUT DATA FRAMEWORK	Substance Property Data Crop Property Data System Data / Boundary Conditions Exposure / Effect Data
FATE PROCESSES FRAMEWORK	Primary Processes Secondary Processes System Loss Processes
MASS COMPUTATION FRAMEWORK	Matrix Framework System Eigendecomposition Mass Conditions (steady state / time *t*) Contributions to System Evolution
EXPOSURE / IMPACT FRAMEWORK	Harvest Fractions Food Processing Factors Direct Intake Fractions Effect Framework (DRFs / ED_{50})
OUTPUT DATA FRAMEWORK	Data Extraction Uncertainty / Sensitivity Framework Evaluation of Results

Characterization Model – Example Results

Health impacts from pesticides applied in EU24 in 2003

crop class	DALY/year
cereals	6.78
maize	3.77
oil seeds	8.82
potato	1.35
sugar beet	0.34
grapes/vines	724
fruit trees	113
vegetables	1100
total	1959 (4.75 to 808,535)

total ≙ 2.6 hours
lost per person
over lifetime

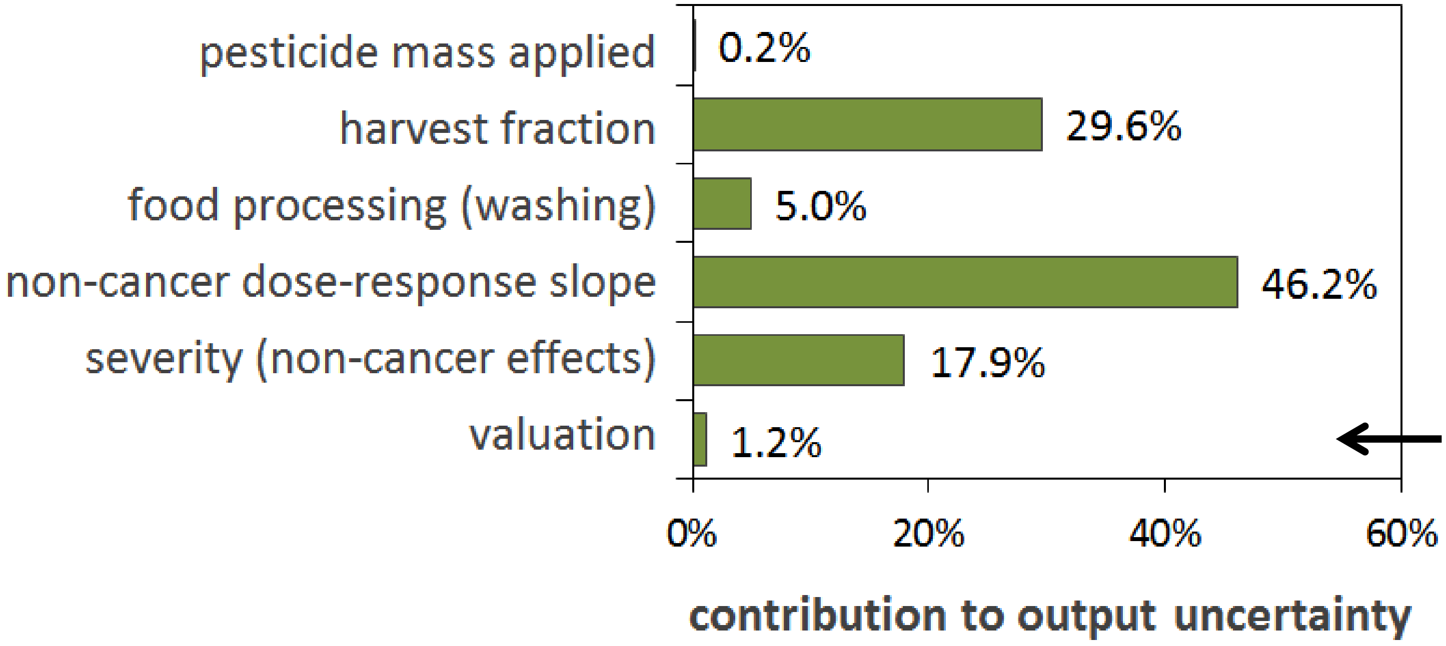
[upper limit: 45 days
per person over
lifetime]

Other stressors (EBoDE Report, 2011)

→ Exposure to particulate matter $PM_{2.5}$: 195 days/person

→ Non-smoker exposure to second-hand smoke: 24 days/person

Characterization Model – Uncertainty



not part of LCIA!

Squared geometric standard deviation (GSD^2) = 428

→ Output uncertainty range: from geomean/428 to geomean×428 (output variability >16 orders of magnitude across pesticides)

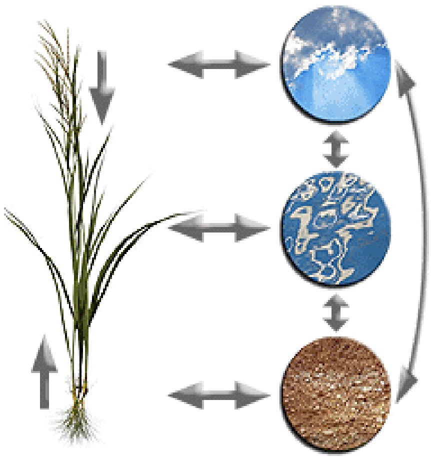
Characterization Model – Limitations

dynamiCROP is so far limited to …

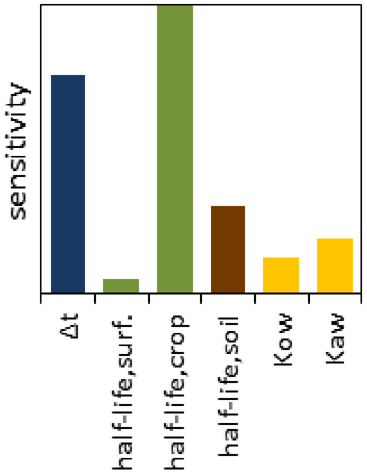
- Assess neutral organic pesticides,
- Assessing parent compounds (metabolites not included in assessment → can be assessed separately),
- Combination of Excel and Matlab (or only Matlab) → parameterized version works without Matlab

Characterization Model – Parameterization

complex model



sensitivity study



regression models

$$y = y^{\text{crop}} + y^{\text{soil}} + \ldots$$

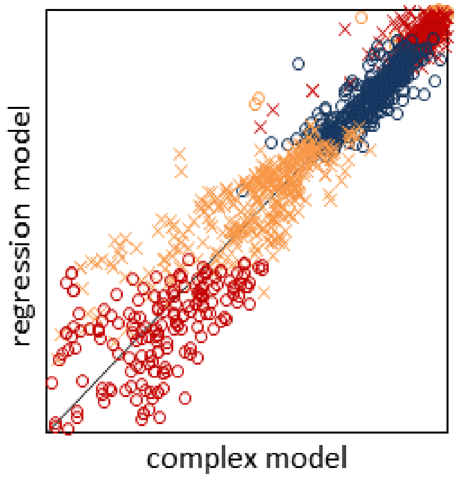
with

$$\log y^{\text{crop}} = \alpha^{\text{crop}} + \beta^{\text{crop}} \times z$$

$$z = f(\Delta t, \text{half-life}, \ldots)$$

...

evaluating results



model parameterization

(factor 4 – 66 mean deviation over harvest fraction range of 10 orders of magnitude)

- Background and scope
- Mass balance system
- From harvest fraction to intake fraction
- Characterization: factors and model
- **Pesticide substitution**
- Highlights and Summary

Pesticide Substitution – Example

Focus (in comparing pesticides): human health impacts

Example crop: wheat

Assumption: all pesticides equally effective

Pesticide Substitution – Target Pests

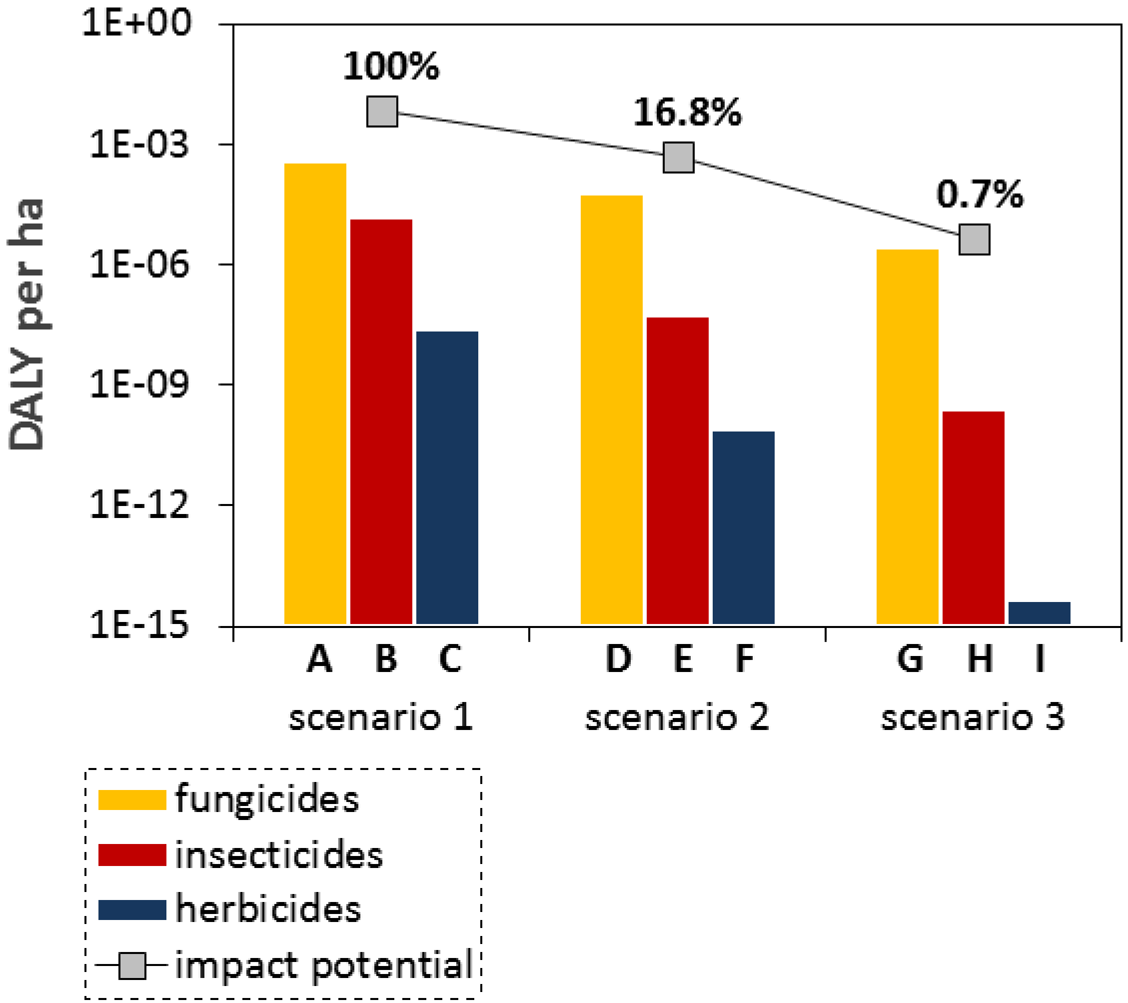
Target pests for wheat as example crop (comparing what?)

- Fungi: e.g. leaf rust, mildew
- Insects: e.g. aphids, thrips
- Weeds: e.g. couch grass, foxtail

Pesticide Substitution – Scenario

	scenario	pesticide	target pests				kg$_{app}$/ha	DALY/ha	DALY/ha	%
insecticides			A	B	C	D				
	1	*β*-cyfluthrin	x	x	x		13.75	2.3E-09	1.5E-06	100
		carbaryl		x	x	x	1.48	1.5E-06		
	2	cyhalothrin	x	x	x	x	0.008	2.6E-09	2.6E-09	0.2
		esfenvalerate		x	x	x	0.012	2.6E-11		
	3	*α*-cypermethrin	x	x	x	x	0.015	2.3E-12	7.3E-12	<0.1
		deltamethrin	x	x	x	x	0.009	5.0E-12		
fungicides			E	F	G	H				
	1	cyproconazole	x	x	x	x	0.08	6.7E-05	6.9E-05	100
		azoxystrobin	x	x	x	x	0.238	2.1E-06		
	2	epoxiconazole	x	x	x	x	0.125	1.3E-05	1.3E-05	18.4
		pyraclostrobin	x	x	x	x	0.175	2.0E-08		
		fenpropimorph		x	x	x	0.45	6.6E-12		
	3	tebuconazole		x		x	0.219	9.7E-09	8.7E-07	1.3
		chlorothalonil	x	x	x		1.5	7.4E-07		
		mancozeb	x	x	x		2.35	1.2E-07		
herbicides			J	K	L	M				
	1	pendimethalin	x	x			1.4	8.7E-12	2.0E-11	100
		fenoxaprop-p	x		x		0.069	1.1E-11		
		prosulfocarb	x	x		x	3.5	1.0E-19		
	2	iodosulfuron		x	x		0.01	7.5E-16	7.6E-16	<0.1
		propoxycarbazone-sodium	x			x	0.05	3.8E-18		
	3	glyphosate	x	x	x	x	1.37	8.8E-22	8.8E-22	<0.1

Pesticide Substitution – Results



fungicides

A : azoxystrobin, cyproconazole

D : epoxyconazole, fenpropimorph, pyraclostrobin

G : chlorothalonil, mancozeb, tebuconazole

insecticides

B : β-cyfluthrin, carbaryl

E : cyhalothrin, esfenvalerate

H : α-cypermethrin, deltamethrin

herbicides

C : fenoxyprop-P, pendimethalin, prosulfocarb

F : glyphosate

I : iodosulfuron, propoxycarbazone-sodium

Pesticide Substitution – Limitations

In reality, substitution must also consider …

- Pesticide authorization (country-specific),
- Crop rotation and climate/soil conditions,
- Pest resistance toward certain pesticides,
- Varying pesticide costs (application count, etc.),
- Other impacts (ecotoxicity, groundwater contamination, etc.)

- Background and scope
- Mass balance system
- From harvest fraction to intake fraction
- Characterization: factors and model
- Pesticide substitution
- **Highlights and Summary**

Highlights

- We are able to characterize health impacts from food crop consumption
- Characterization factors available for 6 crop archetypes and >300 commonly used pesticides
- dynamiCROP model available → dynamic version (matrix-based) and parameterized version (linear, for inclusion in steady state frameworks)
- Highest uncertainties → dose-response and half-lives

Summary

- Exposure of general public to pesticides dominated by residues in food crops
- Lowest residues: root crops, highest residues: leafy crops (wash your salad!), but also fruits and vegetables
- Dynamic assessment required (time to harvest important)
- LCIA helps to compare impacts between pesticides and between stressors (pesticide health impacts low in comparison with e.g. PM → consider uncertainty!)
- Pesticide substitution helps reducing health impacts (other impacts may dominate → include in scenarios!)

Further Information?

- → Fantke, P., Charles, R., de Alencastro, L.F., Friedrich, R., Jolliet, O., 2011. Plant uptake of pesticides and human health: Dynamic modeling of residues in wheat and ingestion intake. Chemosphere 85: 1639-1647.
- → Fantke, P., Juraske, R., Antón, A., Friedrich, R., Jolliet, O., 2011. Dynamic multicrop model to characterize impacts of pesticides in food. Environ Sci Technol 45: 8842-8849.
- → Juraske, R., Fantke, P., Romero Ramírez, A.C., González, A., 2012. Pesticide residue dynamics in passion fruits: Comparing field trial and modeling results. Chemosphere 89: 850-855.
- → Fantke, P., Friedrich, R., Jolliet, O., 2012. Health impact and damage cost assessment of pesticides in Europe. Environ Int 49: 9-17.
- → Fantke, P., Wieland, P., Wannaz, C., Friedrich, R., Jolliet, O., 2013. Dynamics of pesticide uptake into plants: From system functioning to parsimonious modeling. Environ Model Software 40: 316-324.

Contact: **pefan@dtu.dk**