A Dynamic Multicrop Model to Evaluate Pesticides Residues in Food

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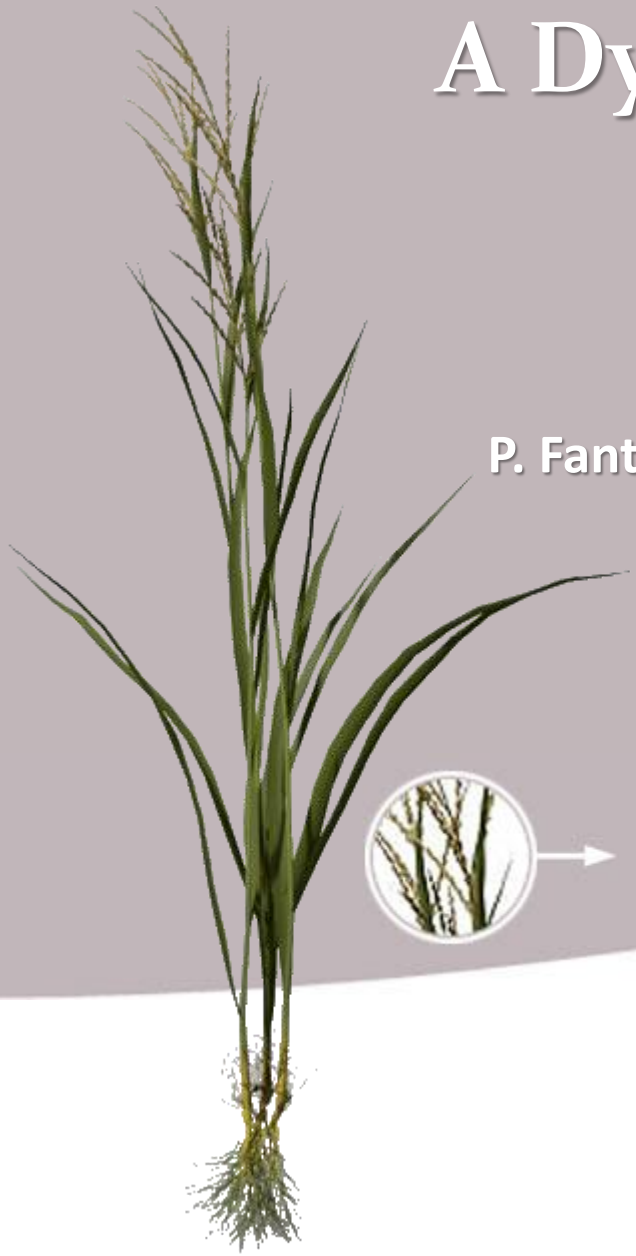

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Outline

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   - Multicrop Aspects
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3. **Parameterization**
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Objectives

Needs ...

- Pesticides residues in various food crops
- Species-specific plant characteristics
- Regression for use in spatial models

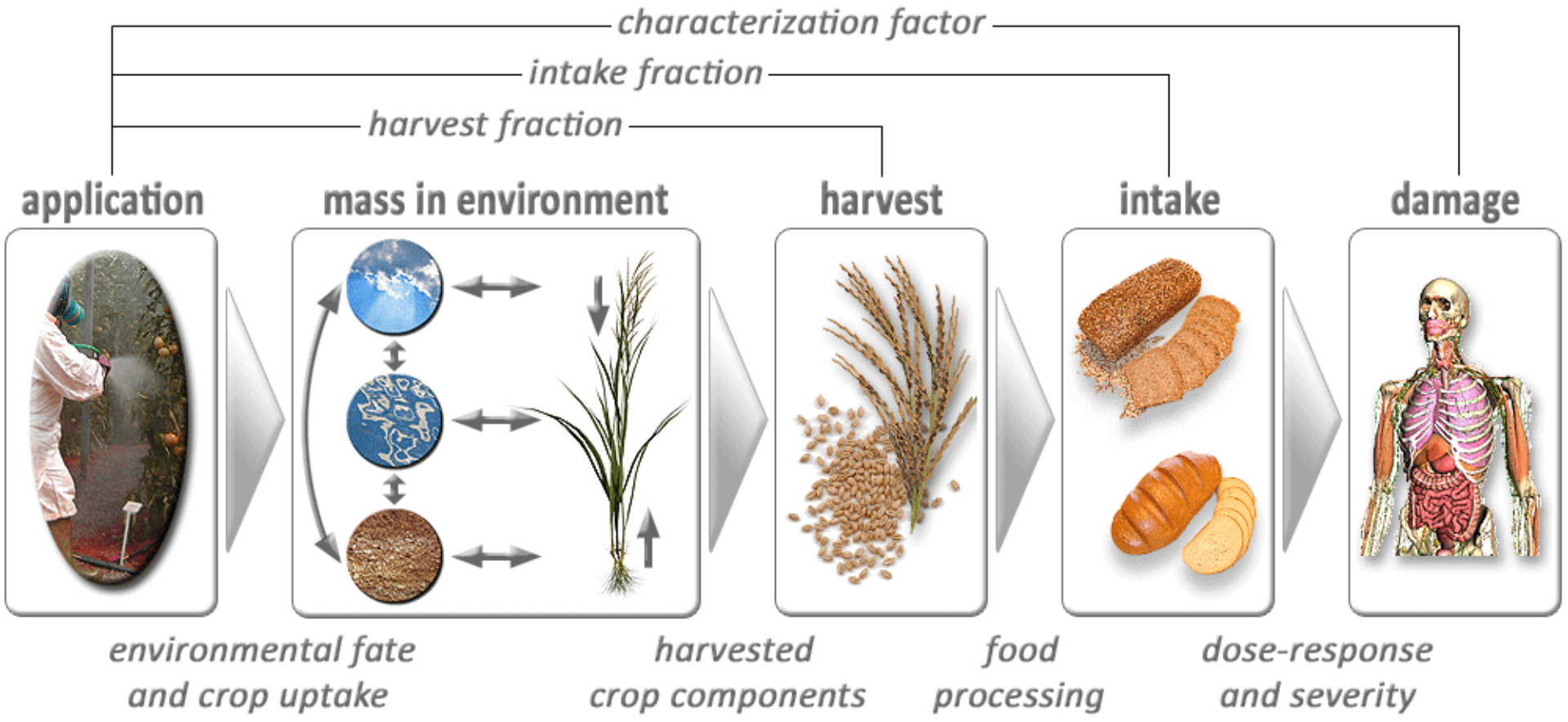
But ...

- No existing multicrop model
- No flexibility for crop-specific aspects
- No model simple enough for integration

Thus ...

- Dynamic crop-specific multicrop model
- Flexible analytical mass balance solution
- System analysis and parameterization

dynamiCROP – Structure



dynamiCROP – Features

System

- Dynamic over time, analytical solution
- Flexible set of connected compartments
- Intermittent character of rain considered

Crop aspects

- Protected (hull) and unprotected fruit
- Exchange between surface and interior
- Logistic growth for stem and root
- Complex growth for leaf area and fruit
- Crop-specific intake fractions

Exposure

- Crop-specific food processing

Multicrop Aspects – 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)

45% of global vegetal consumption

Fantke et al. 2011a (doi: 10.1021/es201989d)

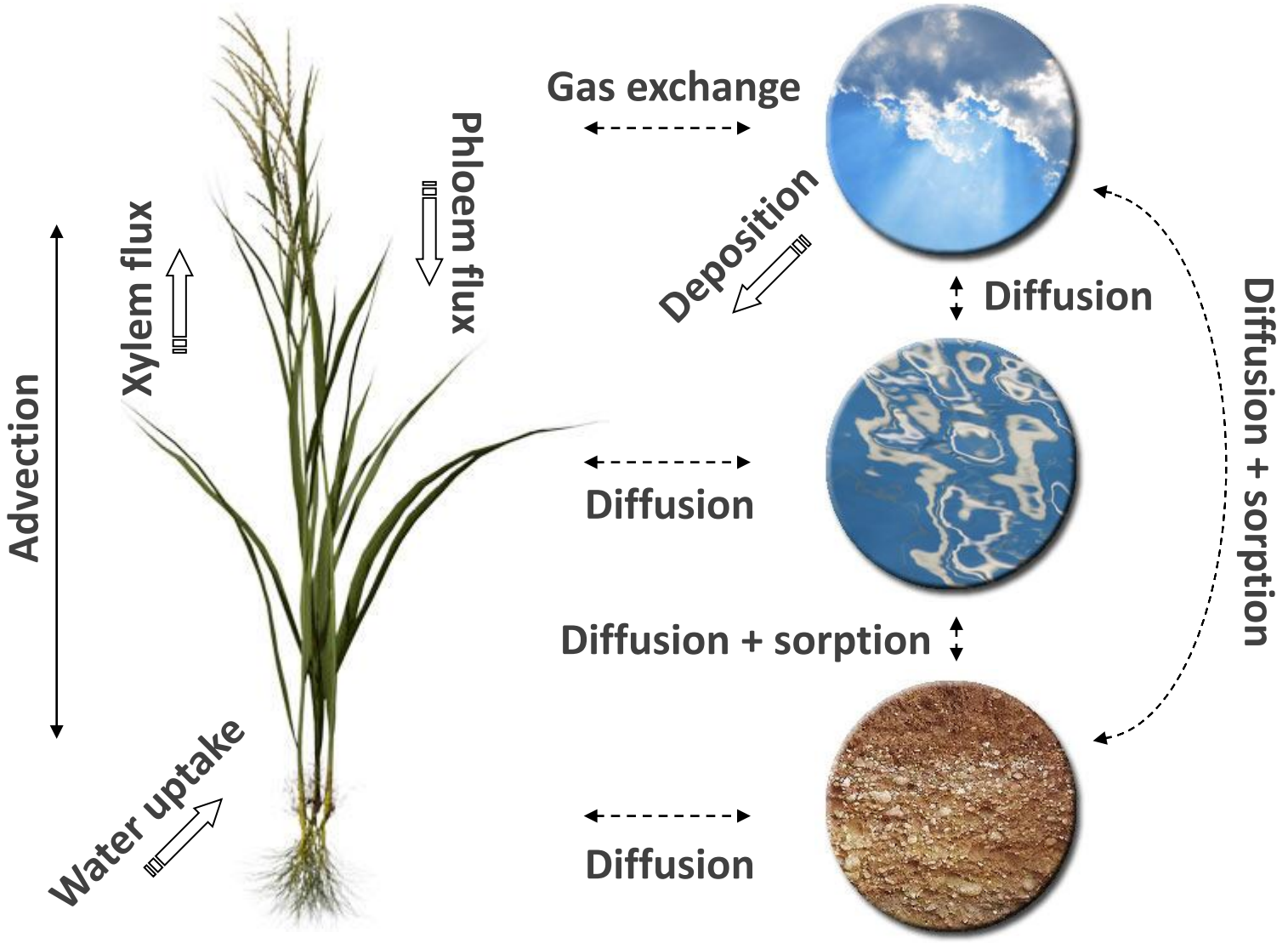
Multicrop Aspects – Criteria

	Residues	Characteristics	Consumed	Models/Experiments
Wheat	medium	grass-like	grain	✓/✓
Paddy rice	medium	grass-like; paddy water	grain	✓/✓
Tomato	high	herbaceous	fruit	✓/✓
Apple	high	tree-like; perennial	fruit	✓/✓
Lettuce	high	herbaceous; high adsorption	leaf	✓/✓
Potato	medium	herbaceous	root/stem tuber	✓/✓

Crop-specific compartment characteristics, processes and food processing considered!

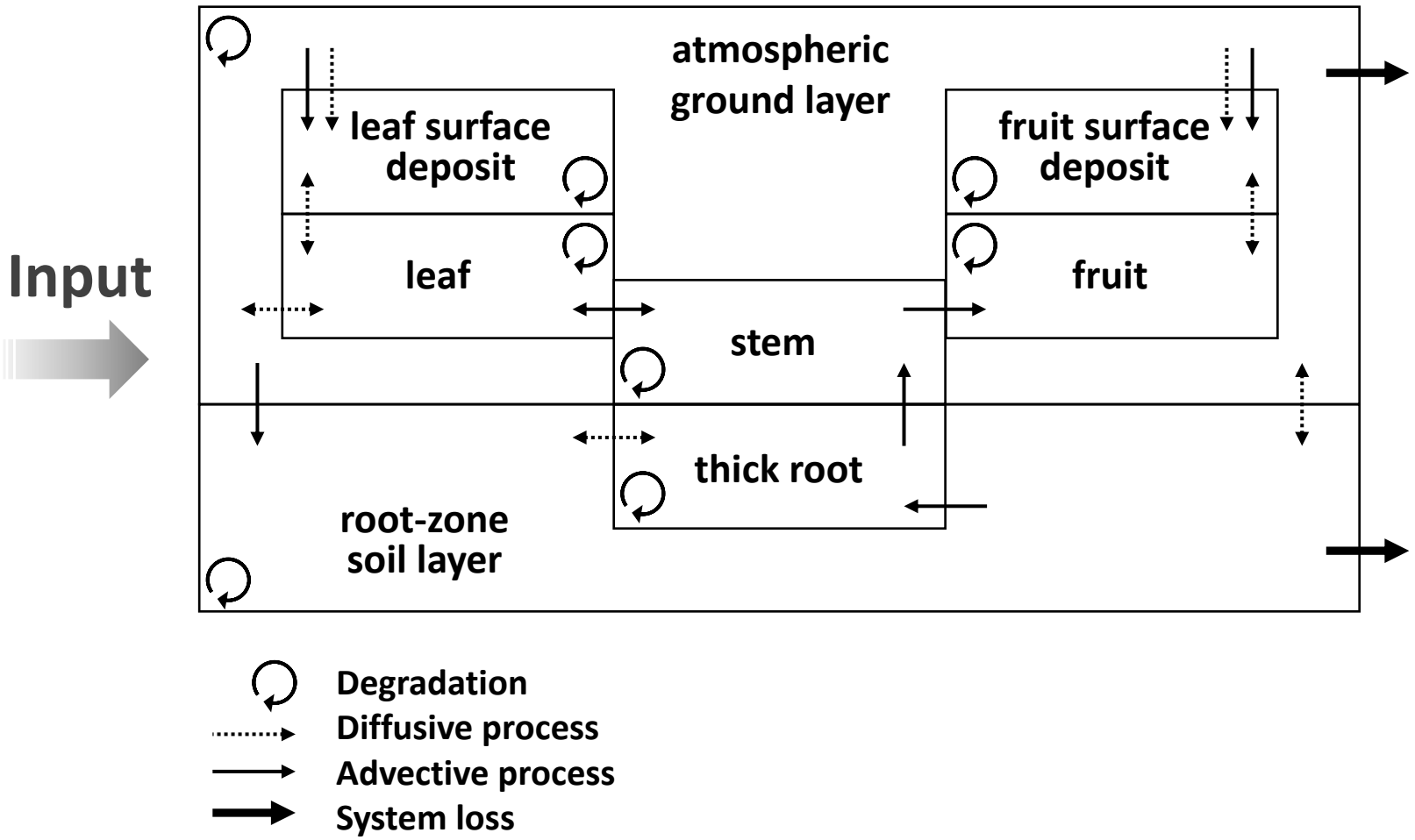
Fantke et al. 2011a (doi: 10.1021/es201989d)

Physical System



Fantke et al. 2011b (doi: 10.1016/j.chemosphere.2011.1008.1030)

Modeled System



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Mass Balance

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

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

$\mathbf{K} :=$

	air	soil	⋯	leaf
air	$-k_{\text{air,total}}$	$k_{\text{air}\leftarrow\text{soil}}$	⋯	$k_{\text{air}\leftarrow\text{leaf}}$
soil	$k_{\text{soil}\leftarrow\text{air}}$	$-k_{\text{soil,total}}$		0
⋮	⋮		⋱	⋮
leaf	$k_{\text{leaf}\leftarrow\text{air}}$	0	⋯	$-k_{\text{leaf,total}}$

Fantke et al. 2011b (doi: 10.1016/j.chemosphere.2011.1008.1030)

Human Exposure

Harvest Fraction residual mass in all harvested crop parts *i* relative to total applied mass

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

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

Intake Fraction mass taken in via consumption relative to total applied mass

$$iF = hF \times PF$$

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

Human Exposure

Harvest Fraction residual mass in all harvested crop parts *i* relative to total applied mass

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

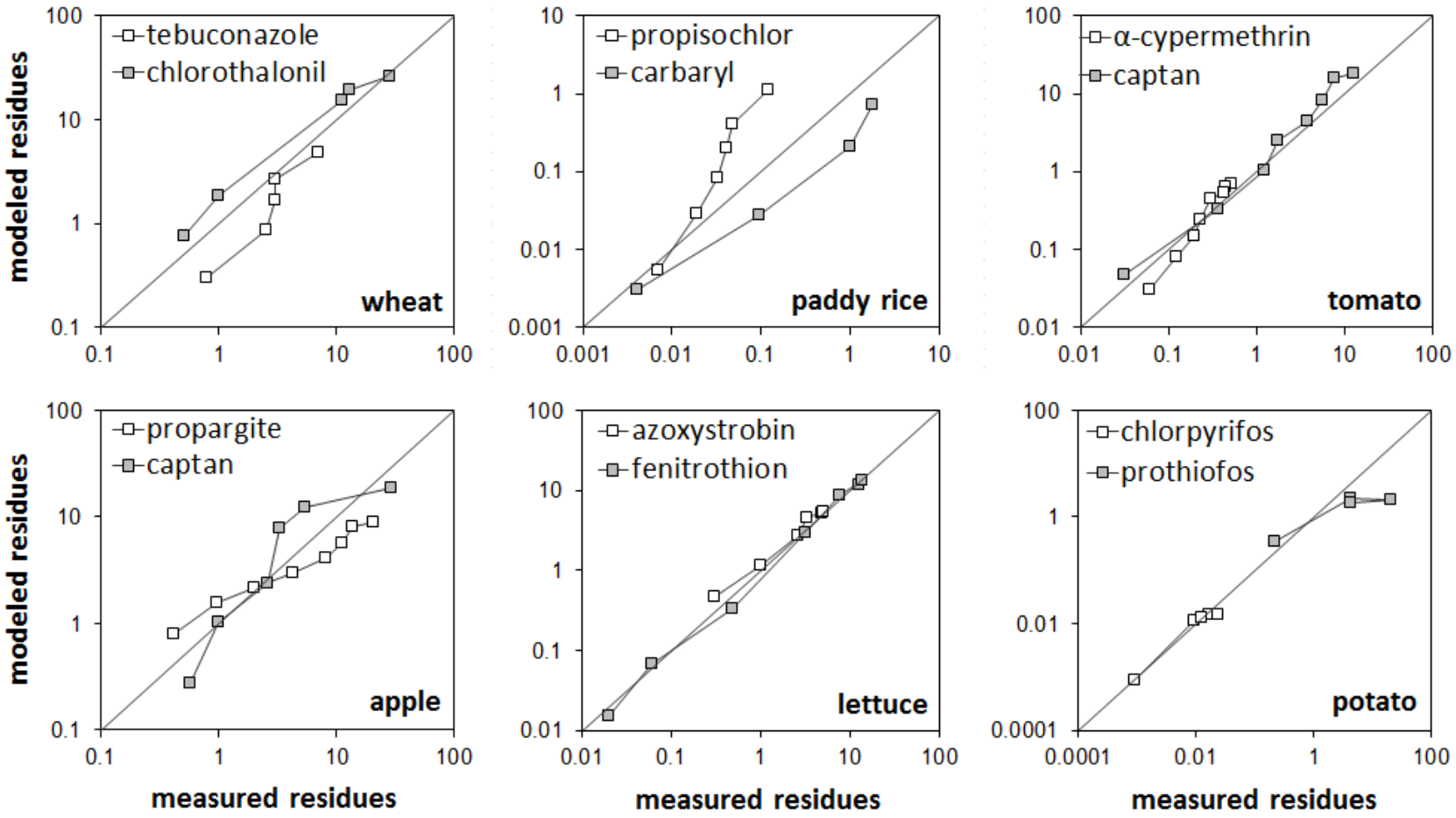
hF	:	harvest fraction [$kg_{in\ harvest}/kg_{applied}$]
m_i	:	residual mass in compartment *i* [$kg_{in\ harvest}$]
m_{app}	:	total applied mass [$kg_{applied}$]
t	:	harvest time [d]

Model parameterization ← **System Analysis**

(reducing complex dynamic model by linear combination of different aspects)

Analysis – Evaluation

Comparison of modeled & experimental residues [mg/kg]



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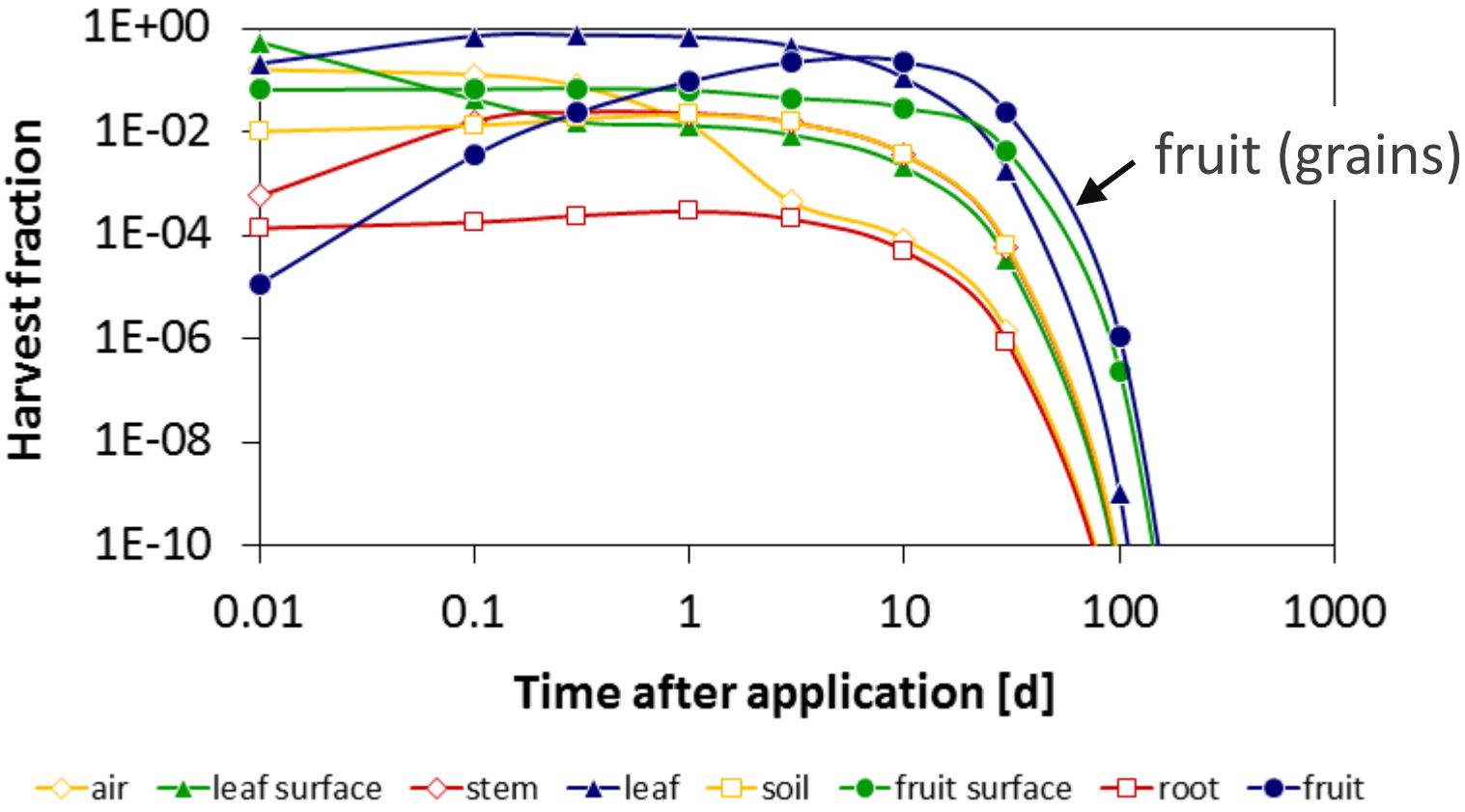
Analysis – Compartments

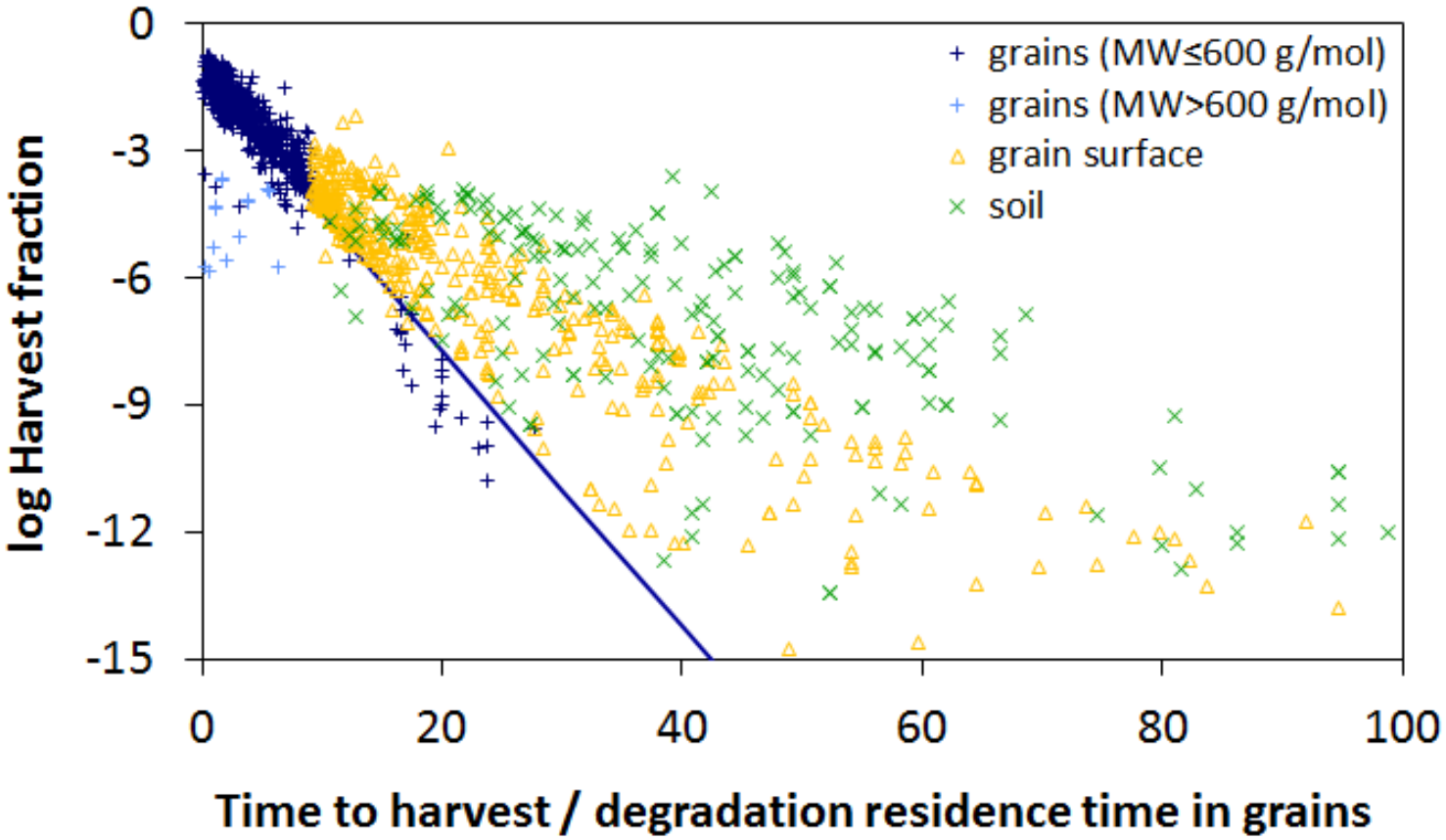
Example: cyromazine (CAS: 66215-27-8) sprayed on wheat



Fantke et al. 2011c (EMS, *submitted*)

Analysis – Other Aspects

385 pesticides sprayed on wheat at **4 different times** (*n*=1540)



Fantke et al. 2011c (EMS, *submitted*)

Regression – Equation

Linear combination

$$hF = hF'_{\text{grain}} + hF'_{\text{grain-surface}} + hF'_{\text{soil}}$$

hF	: harvest fraction [$kg_{\text{in harvest}}/kg_{\text{applied}}$]
α,β	: regression coefficients
t	: time to harvest [d]
HL	: degradation half-life [d]
τ	: degradation residence time [d]
MW	: molecular weight [g/mol]

with

$$\log(hF'_{\text{grain}}) = \alpha_{\text{grain}} + \beta_{\text{grain}} \frac{t}{HL_{\text{grain}}/\ln(2)} + \beta_{\text{MW}}(MW - MW_0)$$

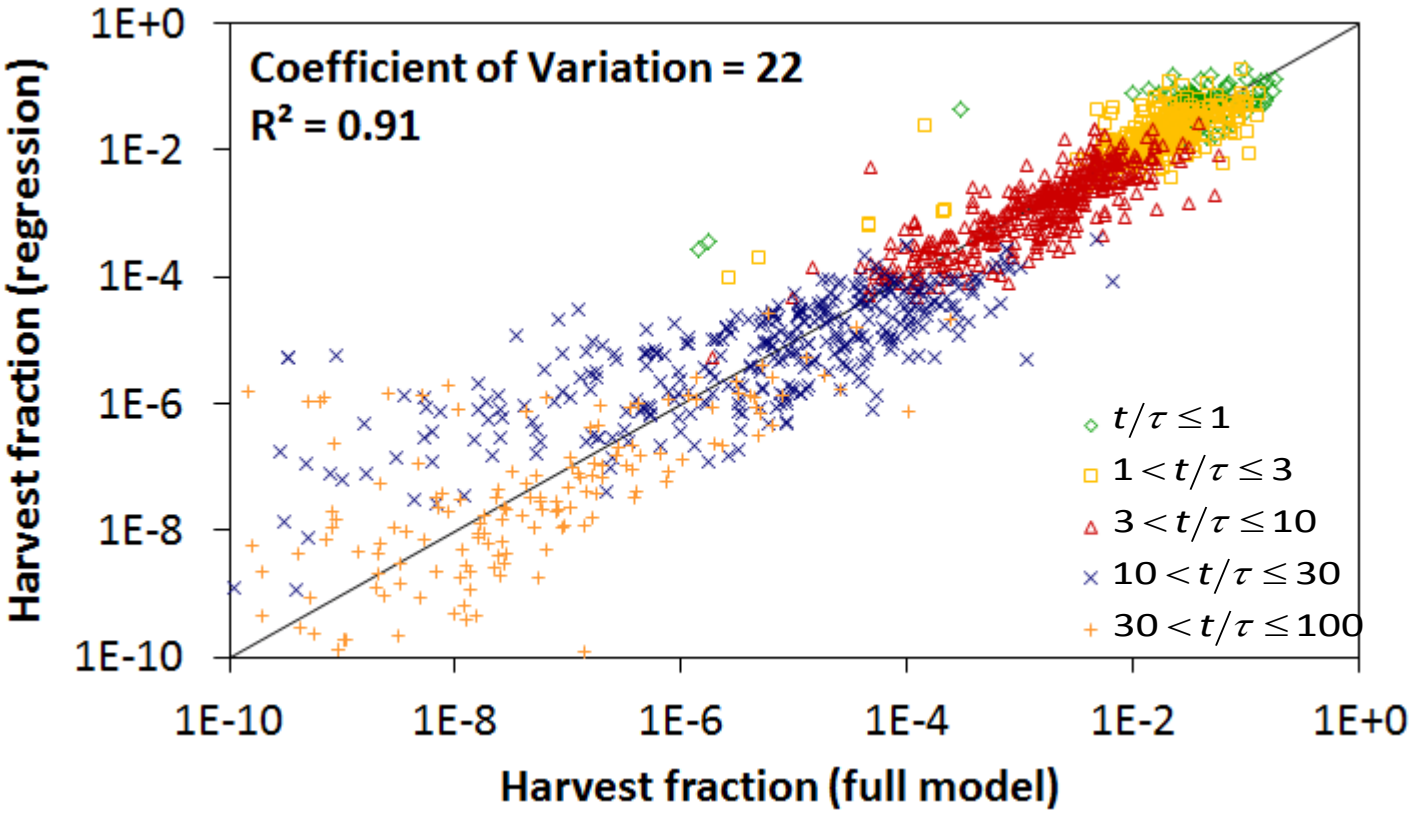
$$\log(hF'_{\text{grain-surface}}) = \alpha_{\text{grain-surface}} + \beta_{\text{grain-surface}} \frac{t}{HL_{\text{grain-surface}}/\ln(2)} + \beta_{\text{MW}}(MW - MW_0)$$

$$\log(hF'_{\text{soil}}) = \alpha_{\text{soil}} + \beta_{\text{soil}} \frac{t}{\tau_{\text{soil}}} + \beta_{\text{MW}}(MW - MW_0)$$

Fantke et al. 2011c (EMS, *submitted*)

Regression – Results

385 pesticides sprayed on wheat at **4 different times** (*n*=1540)



t : time from application to harvest [d]
τ : degradation residence time in grains [d]

Fantke et al. 2011c (EMS, *submitted*)

Regression – Other Crops

Adoption of regression to other crops requires ...

- **Paddy rice** (paddy water aspects, *Kow*, solubility, etc.)
- **Lettuce** (air/leaf exchange aspects, *Kaw*, rain rate, etc.)
- **Potato** (soil aspects, *Koc*, soil matrix, *pH*, porosity, etc.)

→ **Adjustment of regression!**

Conclusions

dynamiCROP full model

- Crop-specific model for characterizing pesticides residues in multiple crops
- Considered crops cover 45% of global vegetal consumption
- Flexible set of compartments and analytical mass balance allow for systematic analysis of system dynamics

Parameterization

- Regression model for wheat with dependency of only 5 input variables
- Deviation from full model of factor 22 over *hF* range of 10 order of magnitude

Development Team

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Model: http://dynamicrop.org

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