# Using the simulation error in lysimeter evaluations

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# Introduction

Lysimeter/field studies are higher tier studies

give additional information about leaching, which can be used for risk assessments in the registration of pesticides.

# Overview decision tree

**1** simple calculation procedure (no PEARL runs) based on standard dossier

**2**
- refined calculations with sophisticated PEARL-GIS tool
- field/lysimeter experiments
- additional laboratory half-lives

1 m

**3**
- behaviour in water-saturated zone

# Questions

- How should lysimeter studies be interpreted in the framework of pesticide registration in the Netherlands?
- How can expert judgements of lysimeter studies be made more transparent and reproducible?
- How to deal with results from various studies with different results and different qualities?

# Advantages of lysimeterstudies over laboratory studies

- a stronger resemblance to environmental conditions in the field soil
- no significant disturbance of the soil
- possibility to study the fate of pesticides in soil/plant systems
- integration of processes (transformation and leaching)

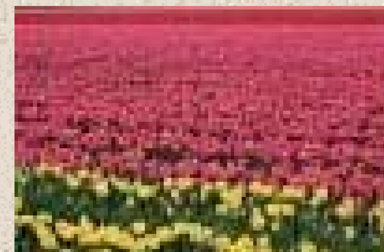
# Advantages of lysimeterstudies over field studies

- the fate of radiolabelled compounds can be measured
- processes of water and solute transport can be studied separately

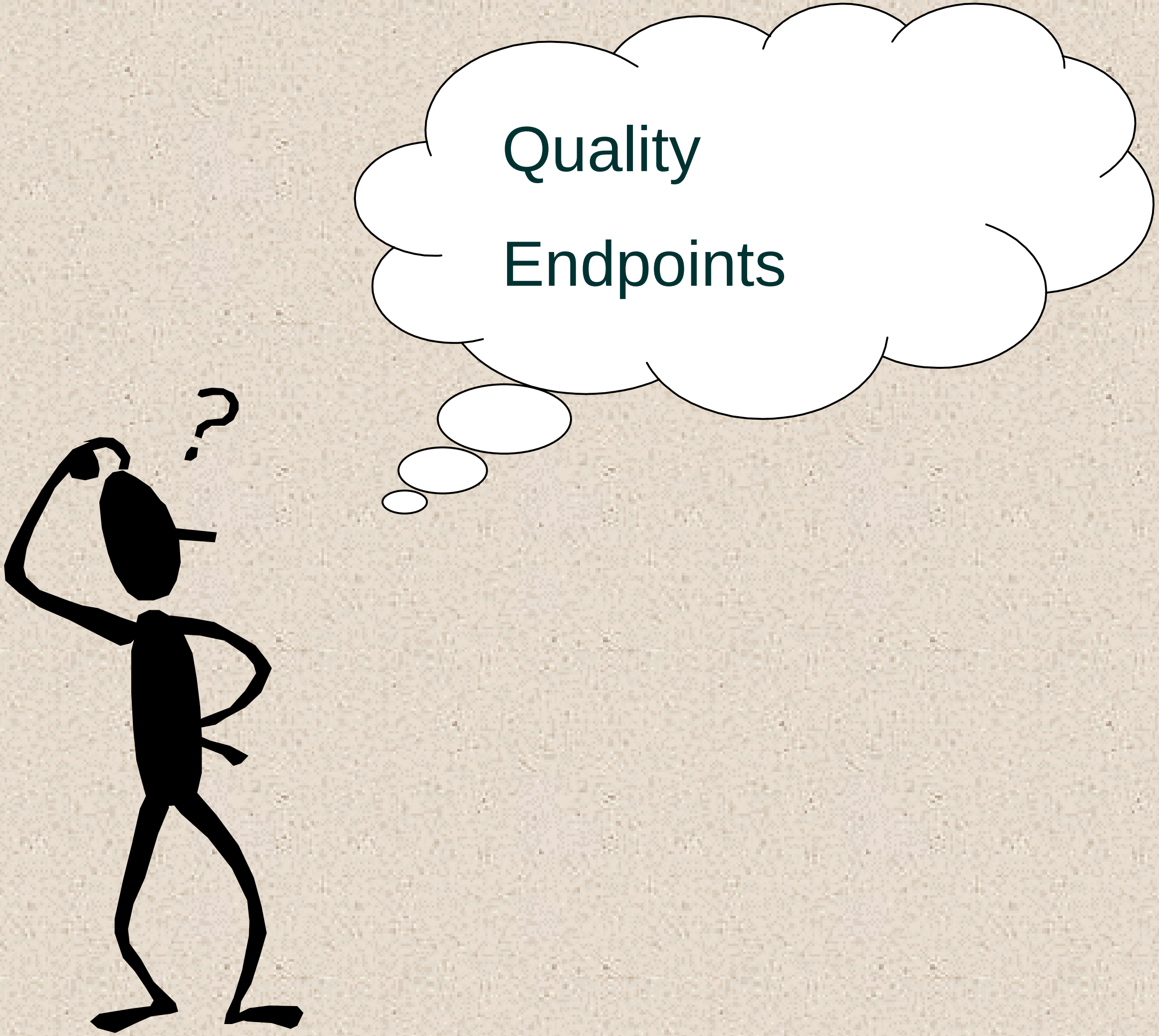
# Advantages of field studies over lysimeter studies

- No edge effects or oasis effects
- The soil profile can be sampled at intervals
- The behaviour of the residues in the groundwater zone can be followed

# Extrapolation to a target scenario



# Expert judgement



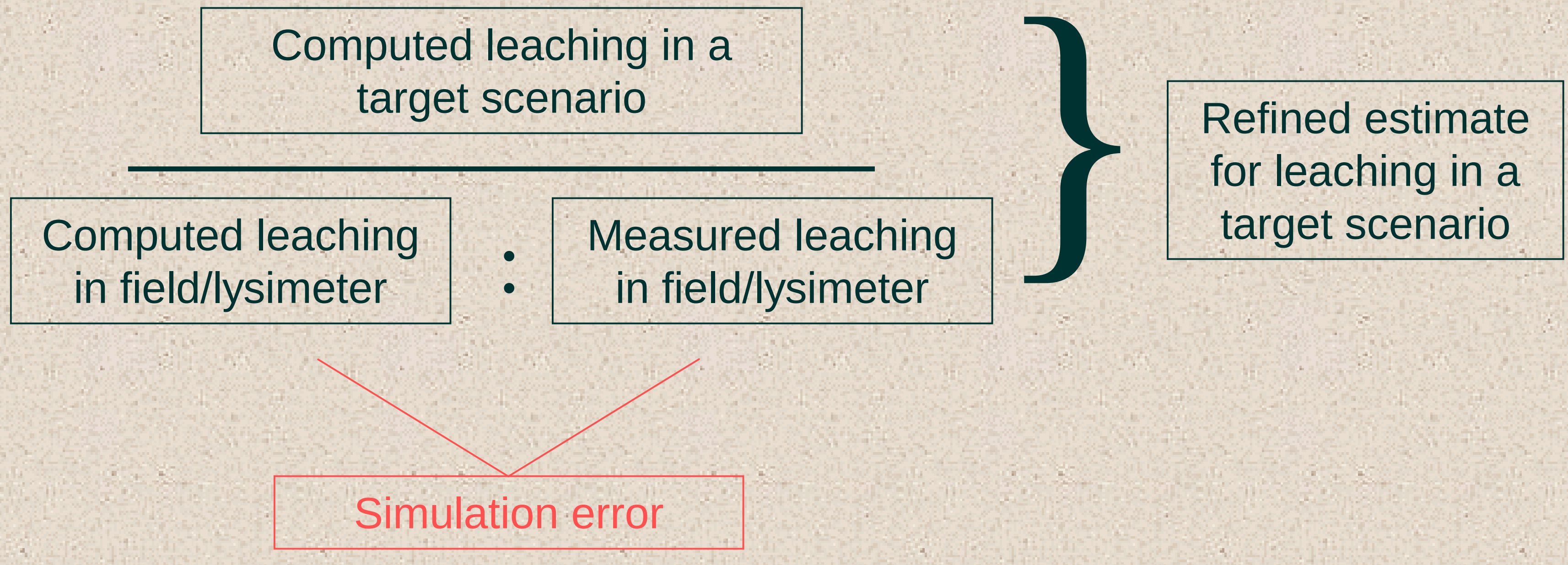
# Endpoints

Compare measurements with simulations

$$E_{SIM} = \frac{C_{field/lys}}{M_{field/lys}}$$

Simulation error is used as correction for simualtion with a target scenario

# Use of the simulation error




A small database with simulation errors can be created

# Simulation errors and the registration

When several field or lysimeter studies are available

a small database with simulation errors can be created

allowing the transparent use of information.

# Simulation input

- Calibration of the water-balance
- Site-specific input, also for DT50 and Kom

No site-specific DT50 and Kom ?
Conservative choices have to be made from dossier values.
= lowest DT50 and the highest Kom

# Checklist for simulation input

| **Item** | **Lysimeter simulation** | **Reliability lower?**[1] |
|---|---|---|
| Soil profile | Lysimeter soil | Q3 |
| no. of layers | according to profile description | Y |
| Depth | at least 1 m | E |
| OM in layers | measured | Q3 |
| pH | measured | For compounds with pKa between 3 and 10 pH dependent sorption can be expected, therefore the pH is essential. If there is no pH given the mobility can not be interpreted →Q3 |
| Meteo<br>Temperature<br>Precipitation<br>solar radiation | At location<br>daily min-max (°C)<br>daily total (mm)<br>measured or calculated | If daily temperatures and precipitation have not been used for the calculations but approximations based on average temperature and precipitation the outcome is indicative →Q3 |
| Water balance | calibrated on amount and pattern of percolation | E. Deviation of 30 mm or 10% of the total amount of water percolated is acceptable. |
| Application scheme | As in lysimeter study | Y |
| Crop | As in lysimeter study | Input parameters of crop should match the crop grown in the lysimeter as good as possible. Estimations based on resemblance to another crops is allowed if the crop is not in the PEARL database. |
| DT50 | From parallel experiment | If the DT50 in the lysimeter soil has not been determined in a parallel experiment, the lowest DT50 from the dossier should be used |
| Kom | From parallel experiment | If the Kom in the lysimeter soil has not been determined it is acceptable to take the highest Kom from the dossier. |
| Duration of simulation | Duration of lysimeter experiment | E |

# Calibration of water balance

| Description | Abbreviation | Unit | Min | Max |
|---|---|---|---|---|
| Soil evaporation parameters: | | | | |
| “Crop factor” for bare soil | FacEvpSol | (-) | 0.5 | 1.5 |
| Parameter in Boesten equation | CofRedEvp | ($cm^{0.5}$) | 0 | 1 |
| Crop parameters: | | | | |
| Extinction coefficient for solar radiation | CofExtRad | (-) | 0 | 2 |
| Min. canopy resistance | RstEvpCrp | ($s.m^{-1}$) | 0 | 1000 |

# Conservative choices

= lowest DT50 and the highest Kom

$$C_{refined} = \frac{C_{rel.scenario}}{E_{sim}}$$

$$E_{SIM} = \frac{C_{field/lys}}{M_{field/lys}}$$

# Simulation error in lysimeter experiments

Comparison of accumulated leaching over the whole study period (kg/ha)

Measurements:

$$Accumulated.Leaching = \sum_{i=1}^{n} V_i \cdot C_i$$

Simulation output in PEARL:

Areic Mass leached

# Simulation error in field experiments

Comparison of concentrations in the upper groundwater at certain sampling times, covering the whole study period (µg/L)

$$E_{SIM} = \frac{\sum_{i=1}^{n} \frac{C_i}{M_i}}{n}$$

# Example field simulation error

| Sampling times | Number of the sampling | Calculated groundwater concentration (μg/L) | Measured groundwater concentration (μg/L) | $C_i/M_i$ |
|---|---|---|---|---|
| 1-I | 1 | 0.000 | <0.02 | ignore |
| 1-II | 2 | 0.000 | 0.03 | 0.000 |
| 1-III | 3 | 0.05 | <0.02 | 2.5 |
| 1-IV | 4 | 0.22 | 0.12 | 1.8 |
| 2-I | 5 | 0.45 | 0.10 | 4.5 |
| 2-II | 6 | 0.53 | <0.02 | 26.5 |
| 2-III | 7 | 0.47 | 0.06 | 7.8 |
| 2-IV | 8 | 0.35 | 0.03 | 11.7 |

Average $E_{sim}$ =7.8

# Quality criteria

- Was the lay-out and experimental set-up adequate?
- Was the soil free of pesticide use in the previous years?
- Was agricultural management in accordance with GAP?
- Are nominal and actual application rates relevant for the intended use of the pesticide?
- Have all the relevant conditions and results been reported?
- Is the method of sampling and analysis valid?
- Is the analytical recovery satisfactory and the limit of quantification relevant for the residues

# Quality classes

Q1: Study is complete, verifiable and reliable and contains all the information needed for interpretation of the results.

Q2: Study does not meet all the requirements, but the most essential data are present.

Q3: Essential information is missing or improper methods have been used. The results can not be interpreted.

# Conclusions

- The simulation error is the endpoint in lysimeter studies
- Site-specific input and calibration of the water balance are essential for a proper calculation of the S.E.
- Information of several lysimeter studies can be joined in a small database
- To obtain a refined estimate for a target scenario the computed leaching for that scenario is divided by the overall S.E.

# Future work

- Calculations with real cases
- Decide upon the choice of the overall S.E. from a small database
- Describe guidance for the calibration of the water balance
- Check/extend the method for metabolites