Guidance for evaluating and using results of field persistence and soil accumulation experiments for exposure assessments

Jos Boesten

EFSA Workgroup Exposure Soil Organisms

Ad-hoc experts
Aaldrik Tiktak (Netherlands Environmental Assessment Agency, NL)
Ciro Gardi (JRC Ispra)
Elena Alonso Prados (INIA, ES)
Jan Vanderborght (Forschungszentrum Jülich, DE)
Richard Bromilow (Rothamsted, UK)

Panel members
Ettore Capri (University of Piacenza, IT)
Jos Boesten (Wageningen UR, NL)
Michael Klein (Fraunhofer Institute, DE)
Ton van der Linden (RIVM, NL)
Walter Steurbaut (University of Gent, BE)

EFSA PPR secretary
Mark Egsmose

Hearing experts
Bernd Gottesbüren (BASF)
Ian Hardy (Batelle)
Ludovic Loiseau (Syngenta)

ppt = draft guidance agreed by workgroup

Outline

- Introduction
- Relevant population of DegT50 values to be considered
- Estimation of DegT50 values from field persistence studies
- Estimation of DegT50 values from soil accumulation studies
- Estimation of mean DegT50 value from combinations of lab and field DegT50 values
- Statistics of public consultation

Introduction

Procedure

- Draft guidance published in summer
- Public consultation until 4 October
- Now: consider all comments and revise guidance
  - adoption end of November
- Then to SCFCAH for taking note

Introduction

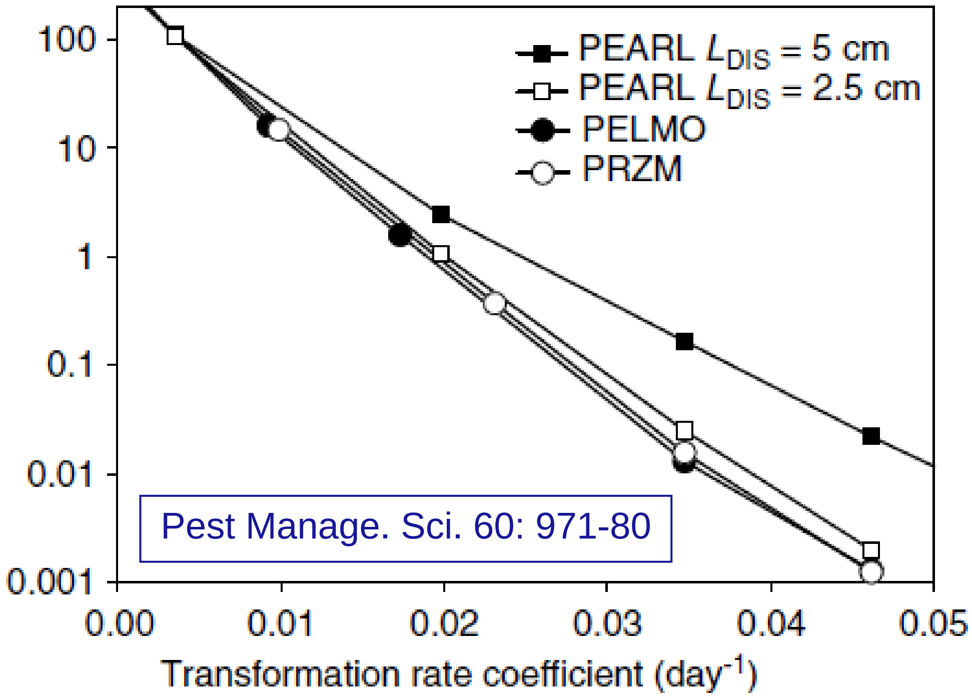
- Problem: how to obtain single DegT50 value for a certain exposure scenario ?
  - DegT50 = for top soil (0-30 cm) at 20^{o}C and field capacity (pF = 2)

- To be used both for scenarios for leaching to groundwater and surface water and for soil exposure
  - different DegT50 values for leaching and soil exposure would be very confusing in regulatory process
  - multi-year simulations including ploughing

- Consequence of use: DegT50 values have to reflect degradation within the soil matrix in top soil
  so surface losses (photodegradation, volatilisation etc.) have to be addressed separately

Introduction

FOCUS leaching concentration (µg/L)



Example: Chateaudun

with K_{OC} = 60 L/kg

Large sensitivity of leaching to DegT50 for FOCUS groundwater scenarios: 15% shorter DegT50 may lead to 50% lower leaching concentrations.

Use of field DegT50 is important aspect of leaching assessment.

Introduction

- First problem: dossier provides a number of DegT50 values but single value needed for each scenario calculation: which type of single value ?

- We want geomean of relevant DegT50 values:
  - FOCUS Degradation Kinetics: geomean of rate coefficients is same as geomean of half-lives
  - EFSA scenario selection for soil exposure was based on median DegT50 (see presentation by Aaldrik) and median is good estimator of geomean for lognormal distribution

Introduction

- Then problem splits into:
  - what is relevant population of lab and/or field studies of DegT50 to be considered for estimating this geomean ?
  - how to estimate an accurate DegT50 from an individual field persistence or soil accumulation study ?
    - considering only spray applications (so no incorporation)
  - how to estimate this geomean DegT50 from combinations of lab and field values ?

Relevant population of lab and field studies of DegT50 to be considered

- Problem: DegT50 as input for a leaching or soil exposure scenario
- What DegT50 values to be considered ?

- Current procedure: accept any ‘normal’ non-vulcanic agricultural temperate soil to estimate DegT50 of any exposure scenario provided that
  - pH, OM and clay are in range of agricultural soils within EU
  - for field persistence experiments: reality check for temperature and rainfall

- E.g. DegT50 (20^{o}C and pF = 2) of Spanish soil with 2% organic matter may be seen as a good predictor for DegT50 (20^{o}C and pF = 2) of Jokioinen soil with 7% OM or Estonian soil with 12% OM

Relevant population of lab and field studies of DegT50 to be considered

- Current procedure is crude: more underpinning needed but also no indications that it is wrong
- Proposal: accept this as working hypothesis but start in parallel activities for testing this hypothesis
  - establish suitable EFSA database
- OECD Ecoregion Crosswalk project has a more subtle approach but has also another aim
  - underpinning will be helpful to communication EFSA-OECD

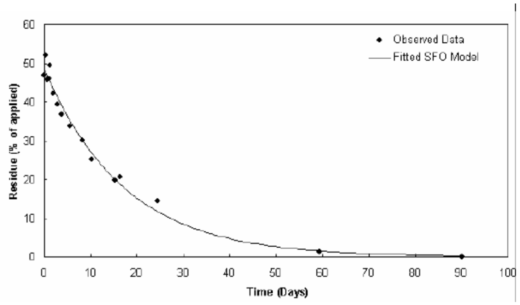
Estimation of DegT50 from field persistence studies

European Food Safety Authority

- Important part of the decline in many field studies takes place in top millimetres
  - 10 cm soil incorporation would make things much better
- Problem 1: find procedure to exclude surface loss processes
- Solution:
  - analyse normalised decline curve with biphasic model
  - use fast phase for estimating initial losses
  - use slow phase for estimation of DegT50
- Problem 2: DegT50 is result of inverse modelling procedure:
  - process descriptions in model may be poor
  - model parameters may be wrong
- Solution: treat field DegT50 values with care, both if they are longer and if they are shorter than laboratory DegT50 values

DegT50 from field persistence studies is result of inverse modelling procedure

measurements **model**



moisture (θ) simulation
temperature (T) simulation
degradation rate simulation

Modelling problems:

- in general poor simulation of θ and T in top millimetres by models such as PEARL and PELMO:

based on constant daily evapotranspiration rate and constant daily air temperature, not considering solar radiation

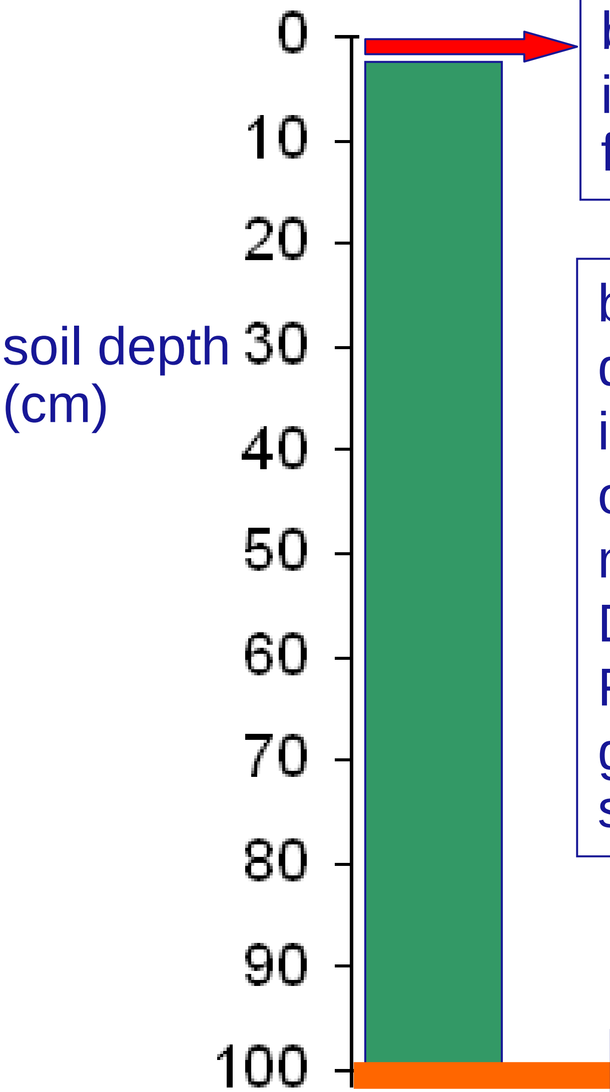
- based on default values of the moisture parameter B and the Arrhenius activation energy E_a

DegT50 from field persistence studies is result of inverse modelling procedure

European Food Safety Authority

- Argument: inverse modelling based on field using the same procedures as for scenario calculations so all possible errors cancel out in scenario calculations
- No studies available to demonstrate this for a range of dossiers
- May be true when considering a large number of dossiers but unlikely to be true for an individual dossiers
- Moreover this cancelling out assumes random effects but for leaching there is an extrapolation problem

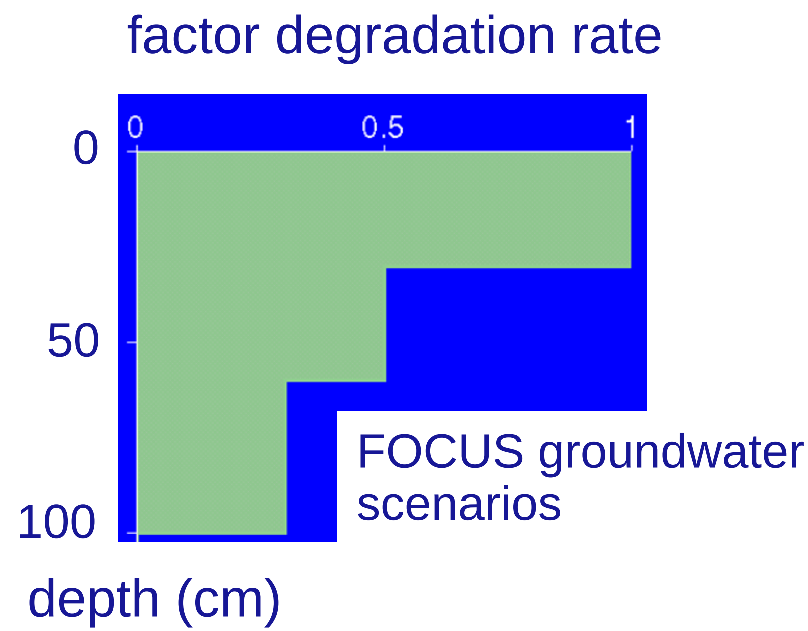
Extrapolation problem when using DegT50 in leaching assessment



behaviour in top cm is main source of inversely modelled DegT50 in many field persistence studies

behaviour in deeper layers is main use of inversely modelled DegT50 in FOCUS groundwater scenarios

evaluation depth



unique relationship assumed for all PPPs in all soils in EU agriculture

Estimation of DegT50 from field persistence studies

- Basis: use normalised decline curves
- Use bi-phasic decline models to separate between surface and matrix processes
- Use either DFOP or Hockey-Stick
  - no FOMC because it does not describe first-order decline in second phase whereas PRZM, PELMO and PEARL assume first-order degradation

Description of DFOP model

$$m = m_{ini}\left(g\ \exp(-k_{fast}\ t) + (1-g)\ \exp(-k_{slow}\ t)\right)$$

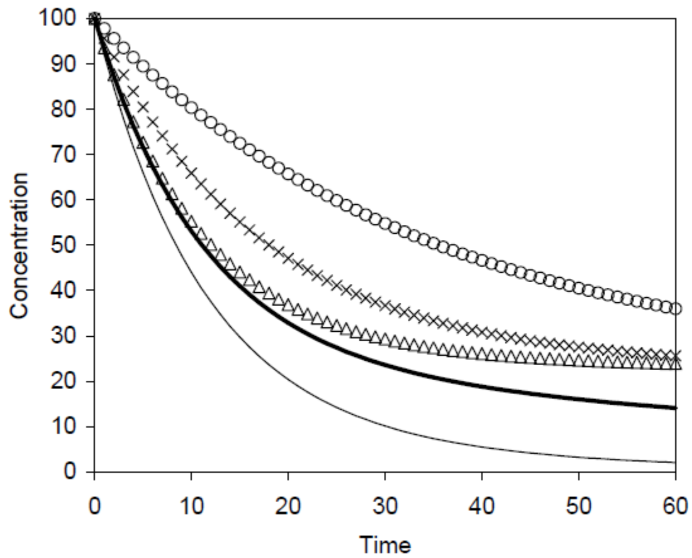
m_{ini} = total mass in system at the start (kg)
g = fraction of total mass in system applied to fastly degrading compartment (-)

k_{fast} = rate coefficient in fastly degrading compartment (d^{-1})
k_{slow} = rate coefficient in slowly degrading compartment (d^{-1})
t = time (d).

we need some breakpoint time to check whether a minimum amount of rain has fallen when slow phase starts:

$$t_b = \frac{3 \ln 2}{k_{fast}}$$

i.e. three half-lives of fast compartment

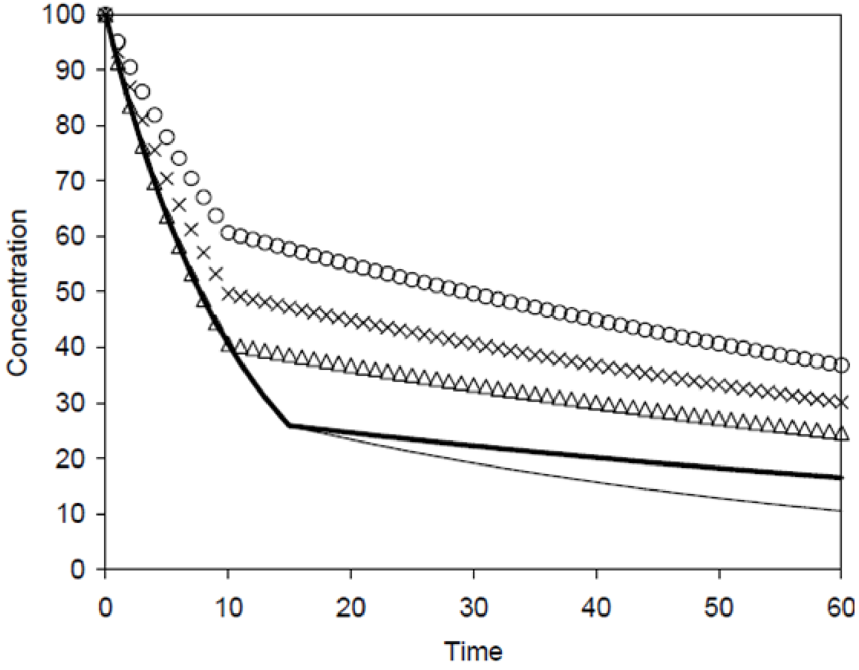


Description of Hockey-Stick model

$$t \le t_b \quad m = m_{ini} \exp(-k_1 t)$$

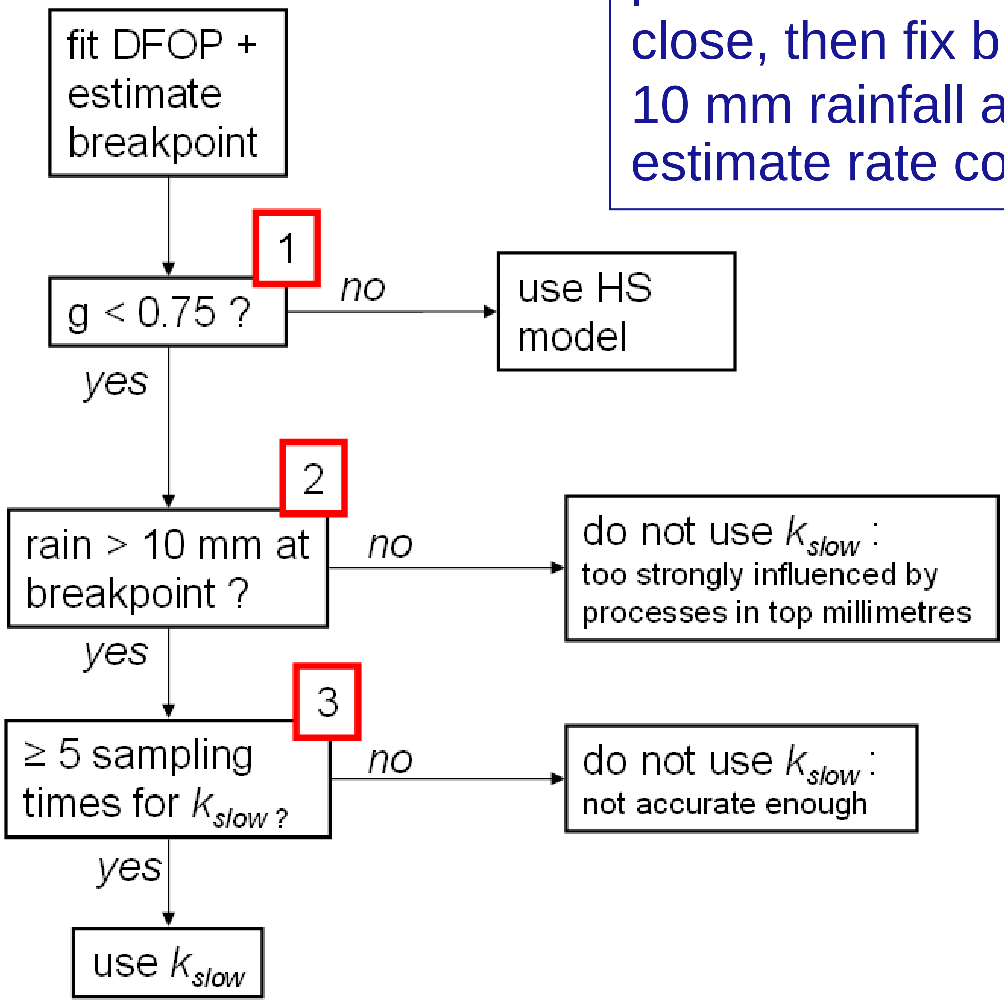
$$t > t_b \quad m = m_{ini} \exp(-k_1 t_b) \exp(-k_2 (t - t_b))$$

t_b = breakpoint time (d)
k_1 = rate coefficient until t_b (d^{-1})
k_2 = rate coefficient after t_b (d^{-1})



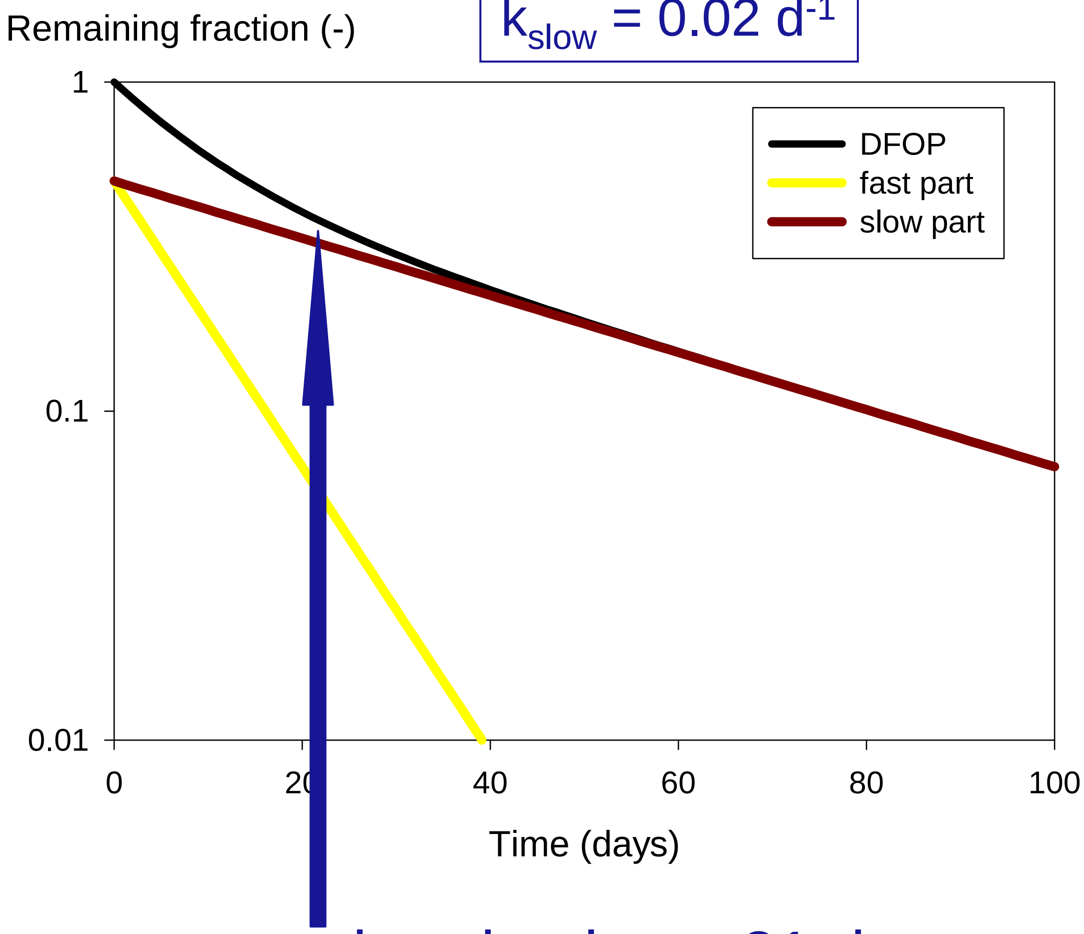
DFOP flow chart

p. 27 : if the two rate coefficients are close, then fix breakpoint at time of 10 mm rainfall and use this to estimate rate coefficients



Explanation of *g*-criterion in DFOP flow chart

k_{fast} = 0.10 d^{-1}
k_{slow} = 0.02 d^{-1}

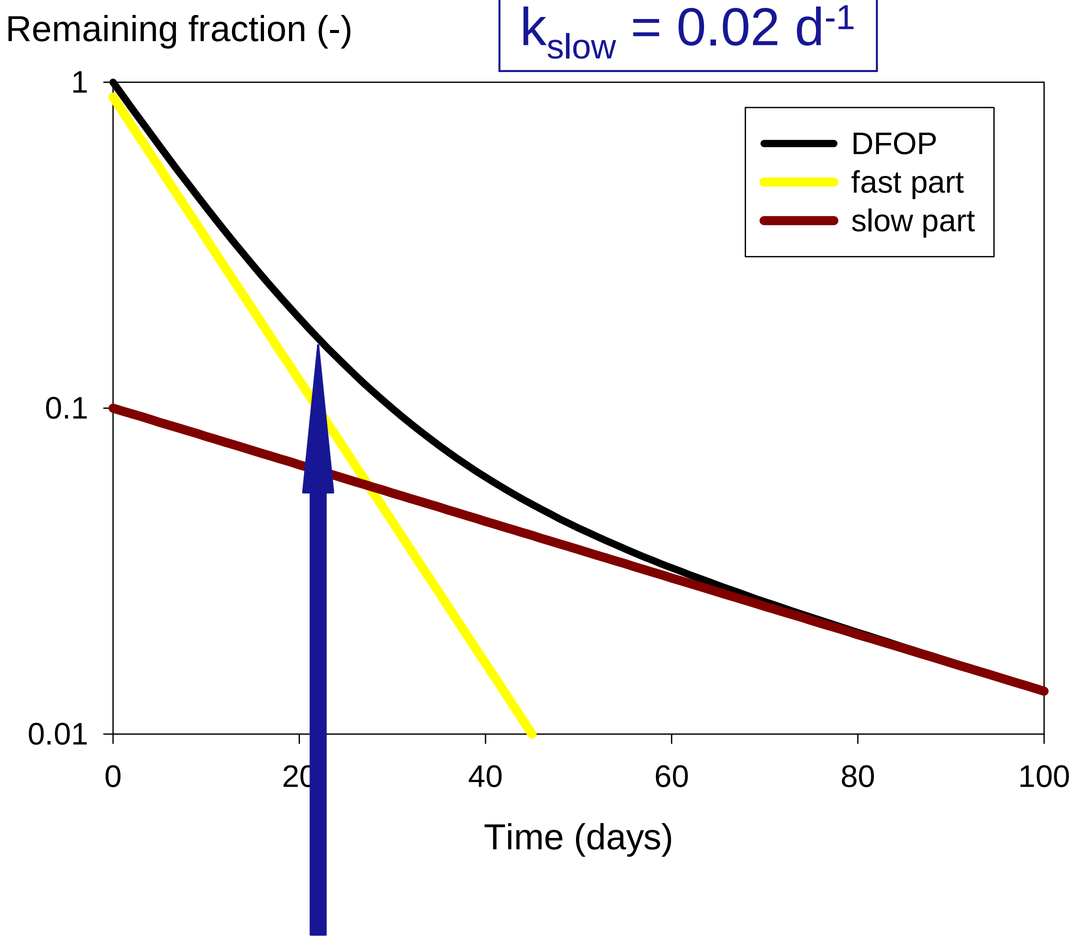


g = 0.5 :
slow phase dominant after breakpoint

breakpoint at 21 d

Explanation of *g*-criterion in DFOP flow chart

k_{fast} = 0.10 d^{-1}
k_{slow} = 0.02 d^{-1}

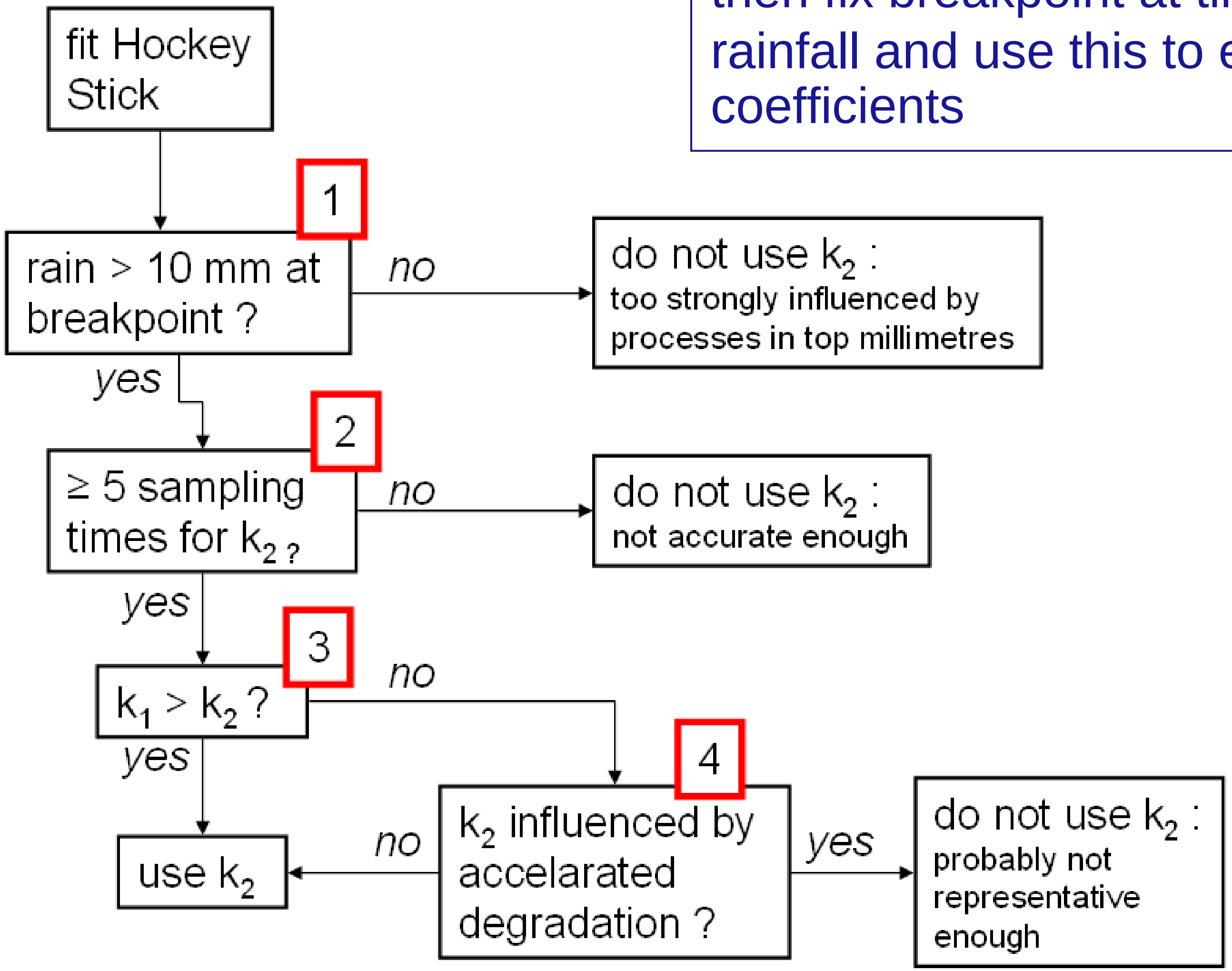


g = 0.9 :
slow phase not dominant after breakpoint

breakpoint at 21 d

Hockey-Stick flow chart

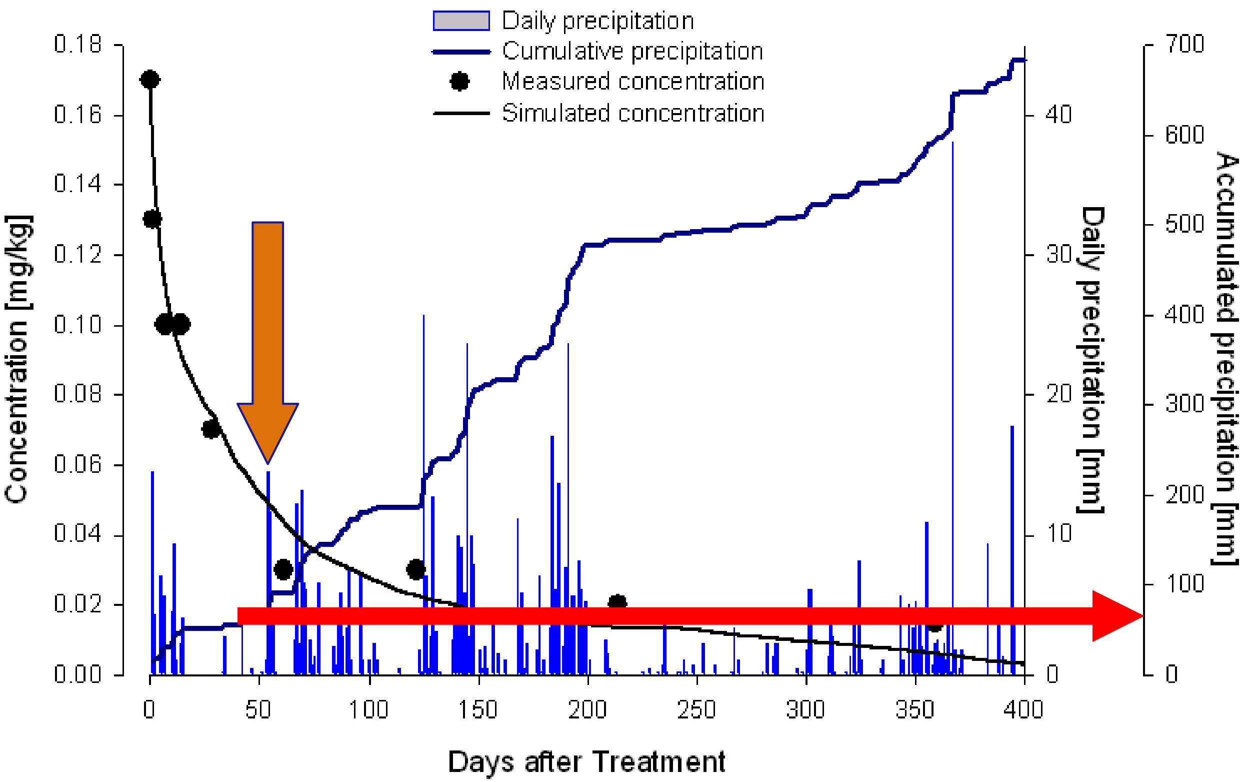
if the two rate coefficients are close, then fix breakpoint at time of 10 mm rainfall and use this to estimate rate coefficients



10 mm stand-alone not enough certainty to exclude surface loss processes

only in combination with biphasic models

background: developing safe criterion too complicated



Application date: June 27, 1990 [END OF FAST DECLINE @ 52 - 92 mm]

pesticide with strong sorption + photochemical half-life of 5 d natural sunlight

personal comm. Bernd Gottesbüren (2009)

Special caution if field is slower than lab

- if a $DegT50_{field}$ is significantly longer than the $DegT50_{lab}$ values then discard $DegT50_{field}$ if it may have been caused by conservative assumptions in the inverse modelling procedure

- Justification: it is unlikely that a lab study with a certain soil would give a shorter DegT50 than a field study with the same soil at the same temperature and moisture content

Estimation of DegT50 from soil accumulation studies

- type-A experiments: two-three samplings per year
  - estimation of fraction that penetrates below the top millimetres in soil separately from DegT50 is impossible with reasonable certainty from such few data
  - do not use such experiments for estimating DegT50
  - spray applications (if incorporated into soil, then no problem)
- type-B experiments: considerably more samplings per year
  - guidance similar to field persistence studies may be used

Estimation of geomean DegT50 from laboratory and field experiments

- Matter of principle in tiered approach:

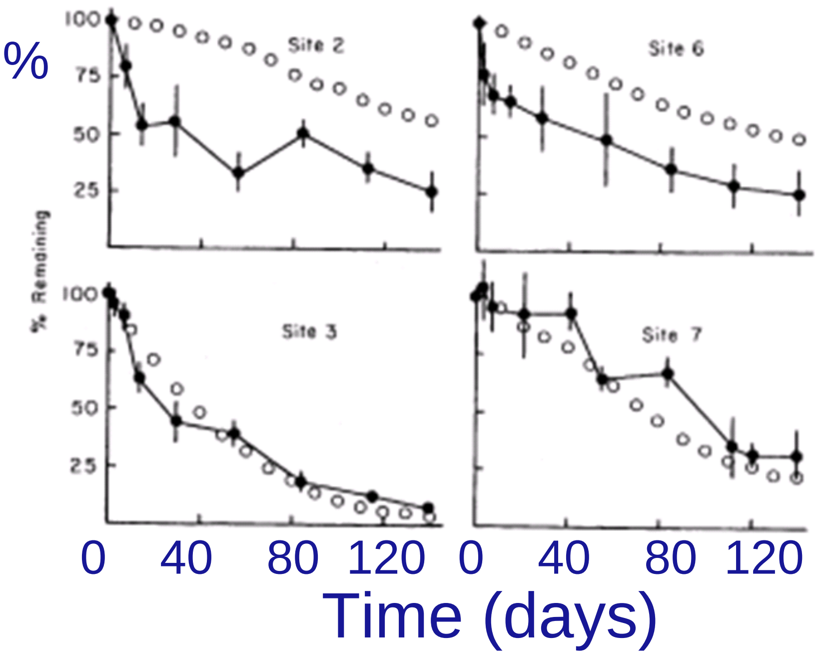
  reject lower-tier data (laboratory DegT50) only if the higher tier provides convincing evidence to justify such a rejection

- A priori, there is no convincing evidence that laboratory DegT50 values are less reliable
  - inversely modelled field DegT50 values have considerable uncertainties for the intended use (especially for leaching)
  - field predictions based on laboratory DegT50 values are often close (next slide)

Can degradation rates in the field be predicted from laboratory studies ?

Examples of field test of the Walker model: comparison of field dissipation of simazine persistence in top soil at 4 sites predicted from lab measurements

Remaining %

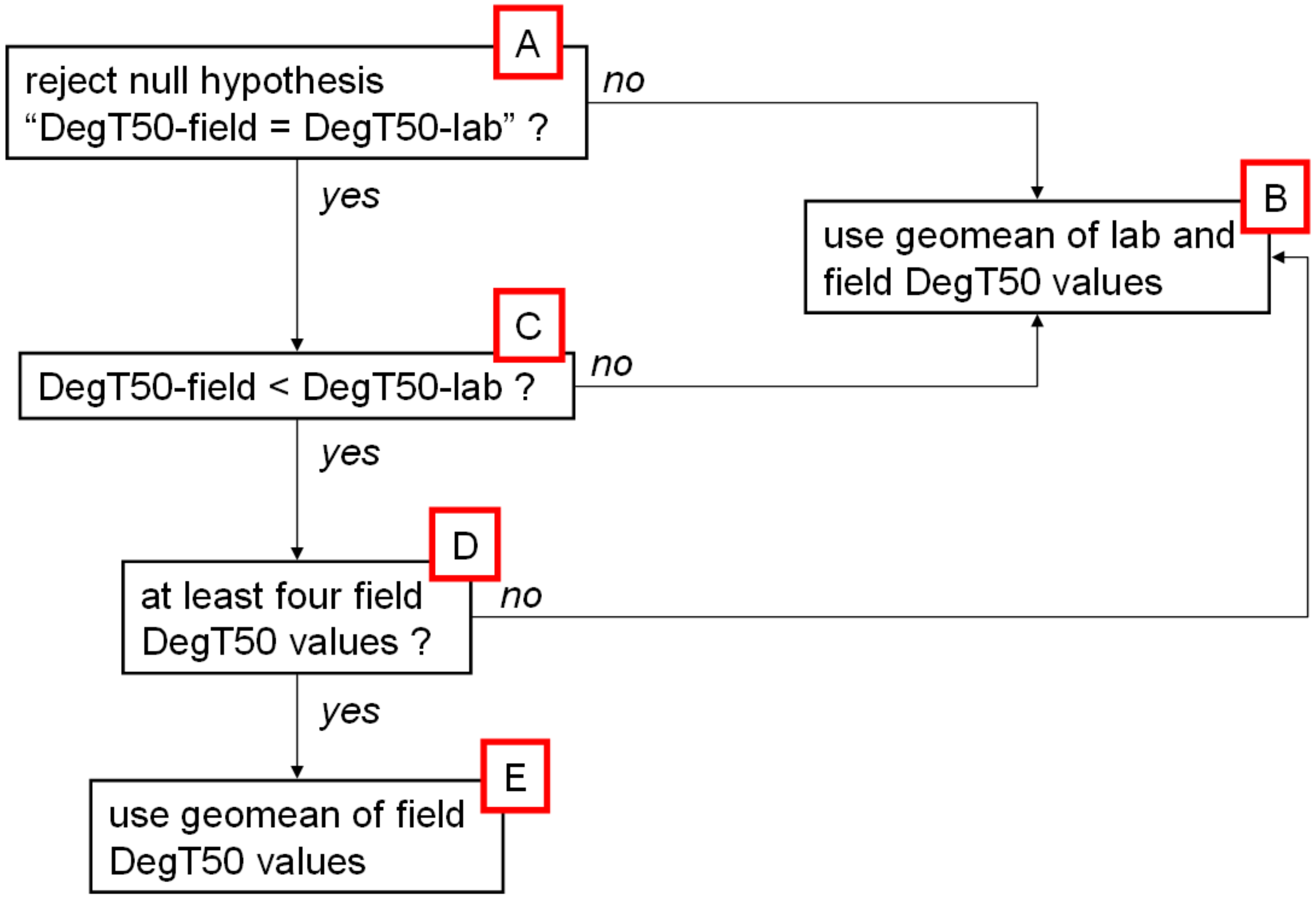


dotted lines: simulated
solid lines: measured

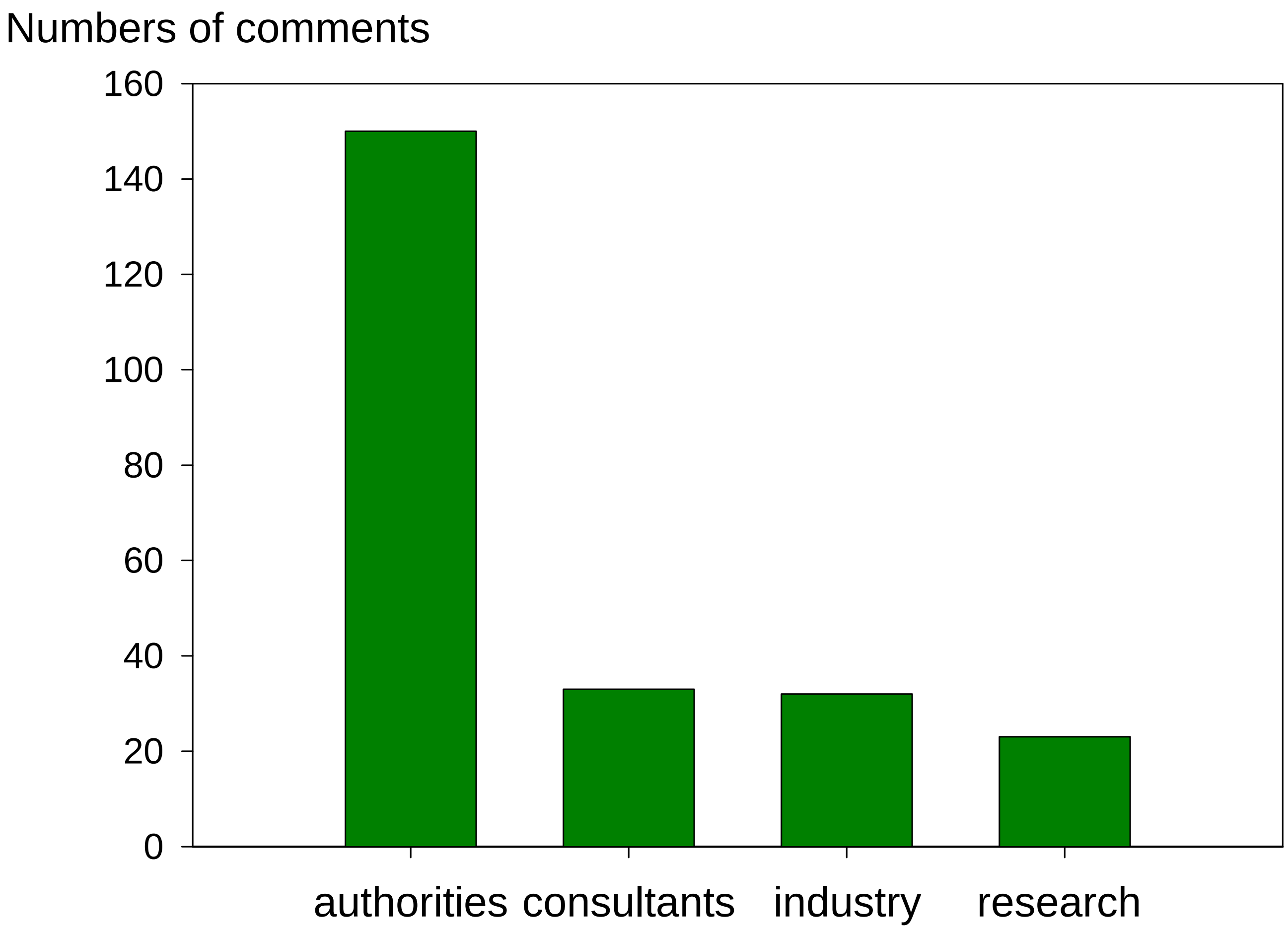
Source: Walker et al. (1983)
Weed Res. 23: 373-83

Such predictions are often close, but may fail to predict either initial rapid declines or (not shown) later fast declines in the field

Estimation of geomean DegT50 from laboratory and field experiments

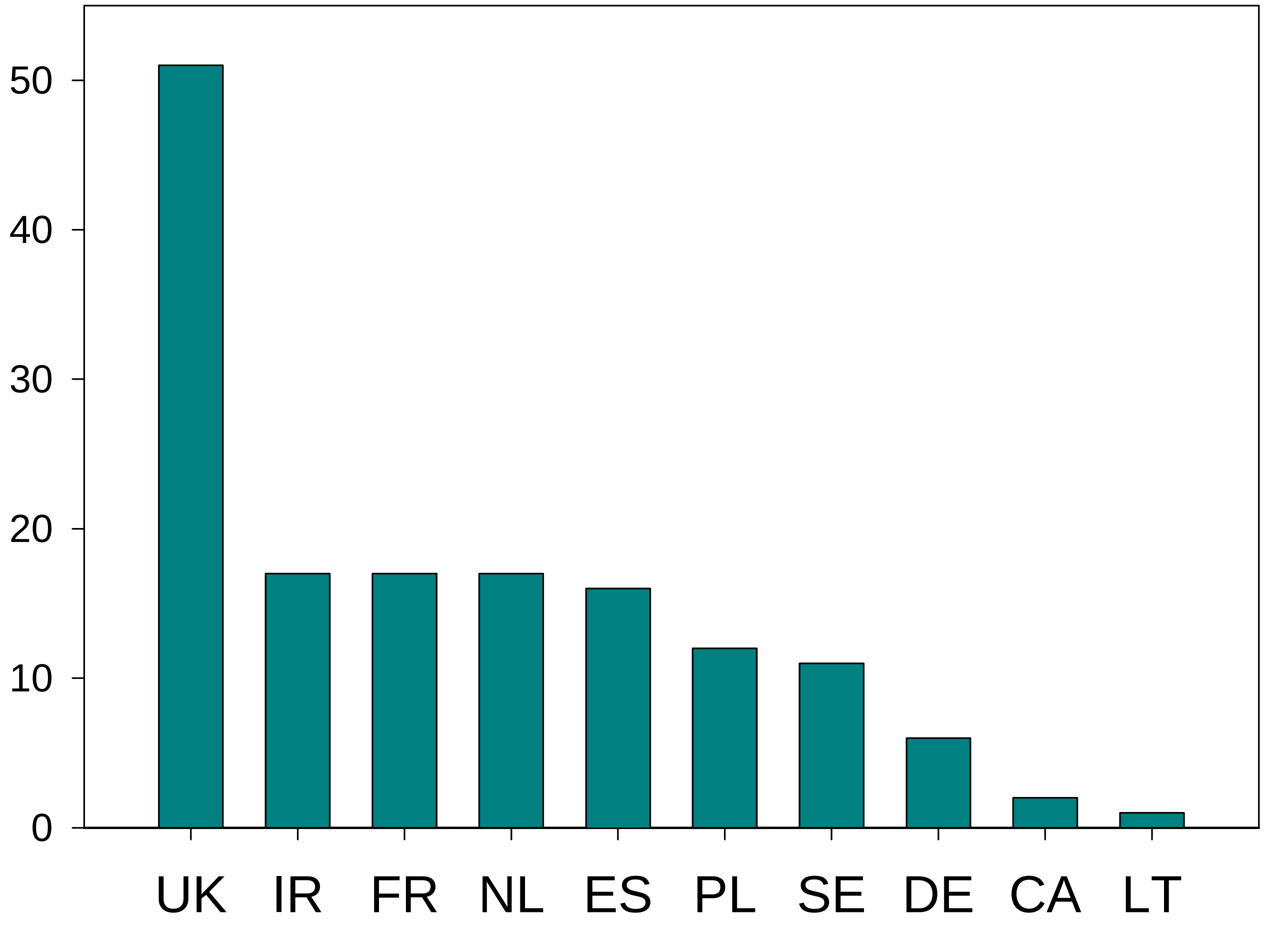


Statistics of public consultation



Statistics of public consultation

Numbers of comments from registration authorities



Thanks !