A briefing document on the application of inverse modelling techniques to pesticide leaching models

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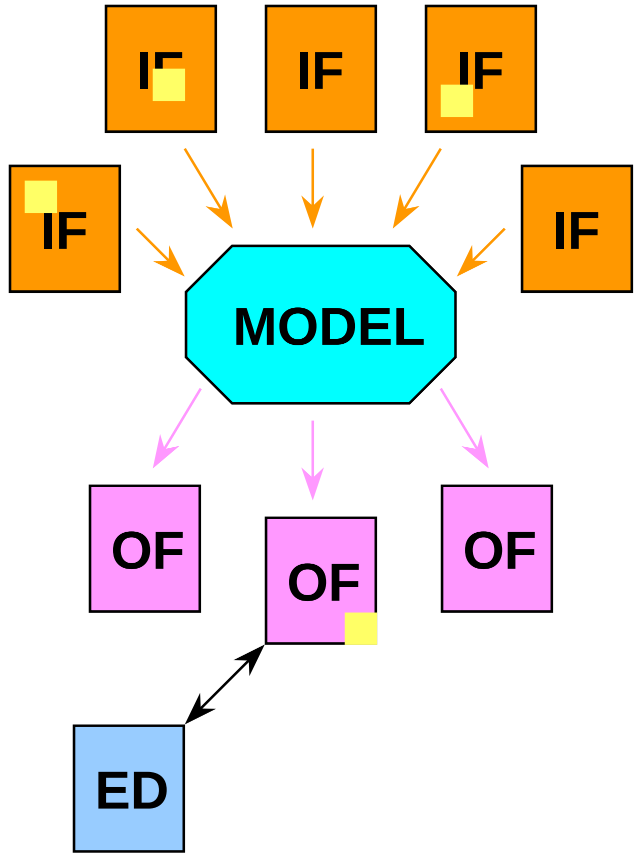
- **Benefits of inverse modelling**
- **Issues associated with inverse modelling**
- **Technicalities**
  - Packages available
  - Overview of the approach
  - When to stop a calibration?
  - Modification of input parameters
- **Two IM examples (MACRO applied to 2 lysimeter datasets)**

Inverse modelling: concepts



General benefits of inverse modelling

- **An alternative to trial-and-error calibration**
  - tedious and time consuming
  - inefficient
  - modification of one parameter at a time
  - criteria for stopping the calibration
  - dependence on user subjectivity

- **Additional benefits**
  - information on the quality of the calibration
  - identification of modelling issues (correlations, sensitivity)
  - model validation
  - advice on model parameterisation
  - better simulation of what happens in the field

Anticipated use of inverse modelling for pesticide leaching models

- **Calibration of models against experimental data**
  - derivation of values for selected parameters (those uncertain)
  - typical examples: water balance ("ET factors", soil, pf)
    solute balance (dispersion)

- **Derivation of sorption and degradation parameters using field data**
  - may be more appropriate than lab and field values for extrapolation
    undisturbed cropped soil
    integrate fluctuating temp and humidity
  - useful for instances where no specific data are available
  - considered as absolute values?

Issues associated with the application of IM to pesticide leaching models (1/4)

- **Ability of the model to describe the field situation**
  - very first assumption!
  - model selection / applicability not to be taken for granted
- **Influence of model and parameterisation**
  - lack of fit because of the model or inadequate parameterisation
  - derivation of lumped parameters
- **Choice of parameters to be included in the modelling exercise**
  - the ones you want!
  - large number of parameters + let the IM package do it
  - influence of parameters not included in the IM
  - combination of sensitivity and uncertainty knowledge

Issues associated with the application of IM to pesticide leaching models (2/4)

- **Influence of starting values on calibration results**
  - IM relies on algorithms which try to minimise the number of runs
  - Greater where large correlations are found
  - Stability of the calibration results

- **Influence of the modeller on calibration results**
  - not known
  - different approaches
  - how does it compare to the other factors?

- **Influence of the inverse modelling package used**

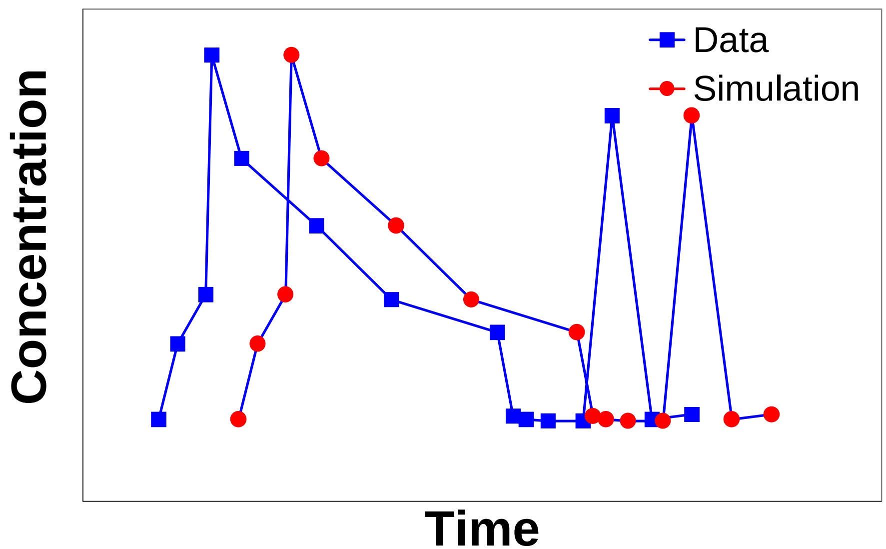
Issues associated with the application of IM to pesticide leaching models (3/4)

- **Influence of the quality of the experimental dataset**
  - minimum number of points required
  - dealing with “zeros”
  - more / less datapoints
- **Comparison between model predictions**
  - Lysimeters: integration in time
  - Suction samplers: integration in space
  - post-processing programs required

Issues associated with the application of IM to pesticide leaching models (4/4)

- **Influence of the attribution of weights**
  - different approaches which can be all justified

- **Numerical vs visual assessment of the GOF**



Conclusions - discussion

- Benefits are potentially significant
- BUT there are also numerous issues to be addressed
- IM requires some serious pre- and post-thinking
- Use of IM in the registration arena: is a calibrated DT50 a DT50?