Minimal variation in input parameters highly influences PEARL and PELMO results: how can these results be trustable?

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The problem

The prediction of the potential **leaching of pesticides into groundwater**, for EU registration purposes, is carried out by **FOCUS models**, in particular by PEARL and PELMO models. Predicted environmental concentrations in groundwater (PEC_{GW}) are influenced by substance specific parameters such as **DT_{50}, K_{OM}** and **Freundlich coefficient** (1/n). Great variations in PEC_{GW} values are expected when a high variability occurs in one or more of the parameters listed above. However, it has to be underlined that PEC_{GW} output could be significatively **affected also by minimal variations** of the same parameters. Considering that minimal variations are intrinsic in laboratory studies, a corresponding high variation in the model results is not scientifically acceptable.

Description of the project

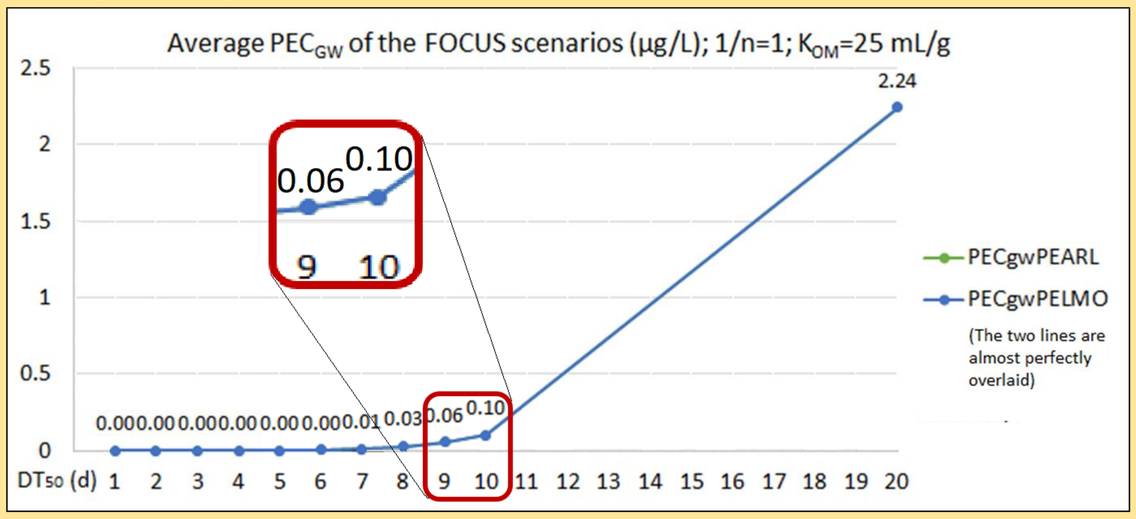
PEC_{GW} calculations have been performed on **808 dummy substances** with various combinations of DT_{50}, K_{OM} and 1/n values, to examine the influence of each single parameter on the final result, and to analyze the **sensitivity of PEARL and PELMO models** to these variations. Other active substance characteristics and the application scheme (1x1000 g/ha each year, spray application on soil surface at 10 d before emergence of maize crop) were kept constant for all the substances. The results obtained were used to create a **classification system** for the input parameters K_{OM} and DT_{50} according to the models sensitivity. Furthermore, experimental uncertainty intrinsic in the parameters determination was analysed and taken into account to refine the classification system. **Conservative values** for each parameter class, to be used in PEC_{GW} calculations, are proposed for all substances. This approach is expected to minimise the effects of the intrinsic input variability providing a better scientific approach to the assessment of groundwater modelling in the regulatory context.

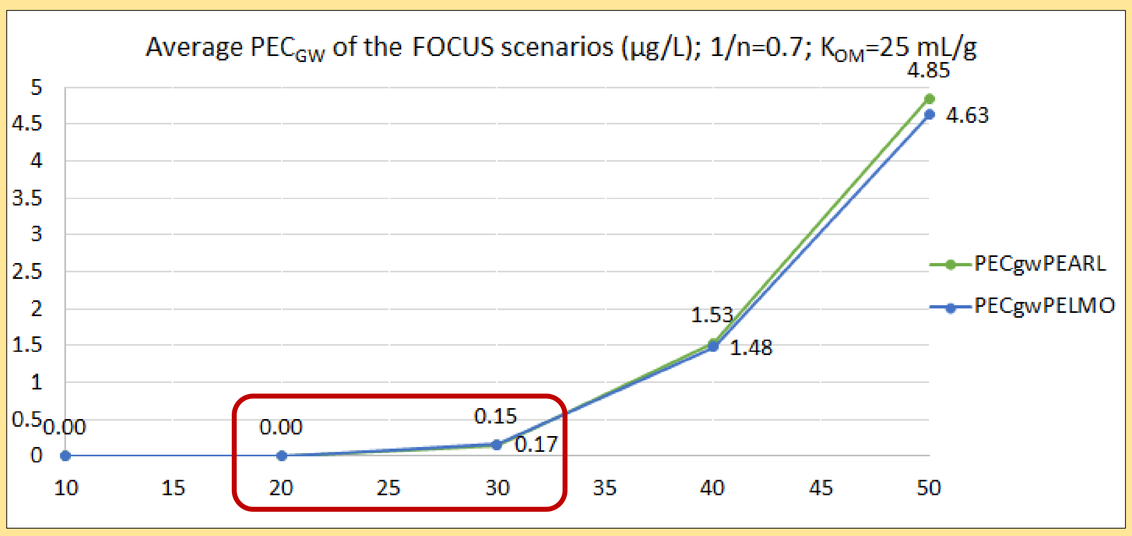
DT_{50} variation

K_{OM} (mL/g): 25, 100, 325, 1250, 3500 1/n: 0.7, 0.8, 0.9, 1

DT_{50} (d): 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500.

Examples of significative variations:



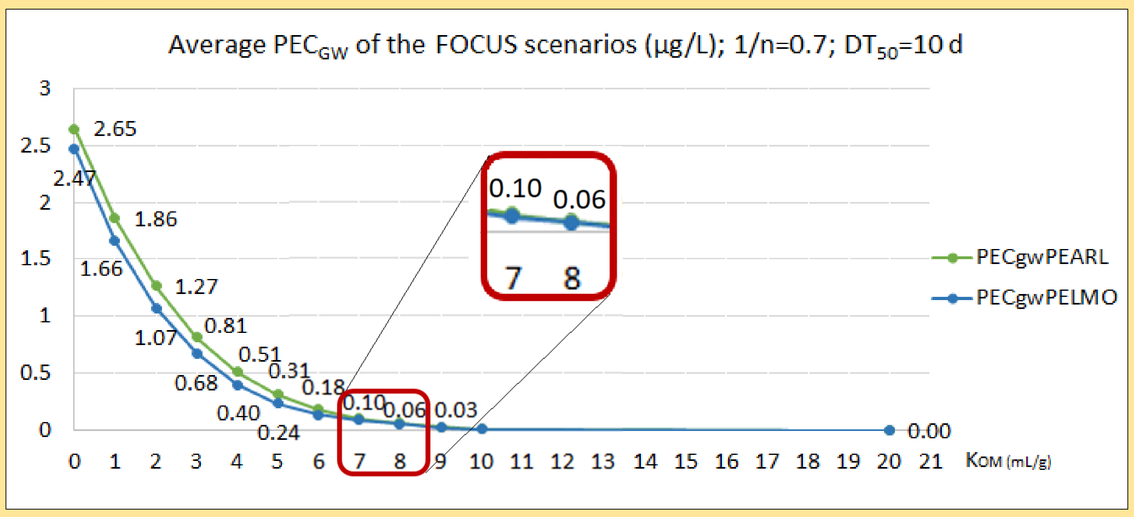


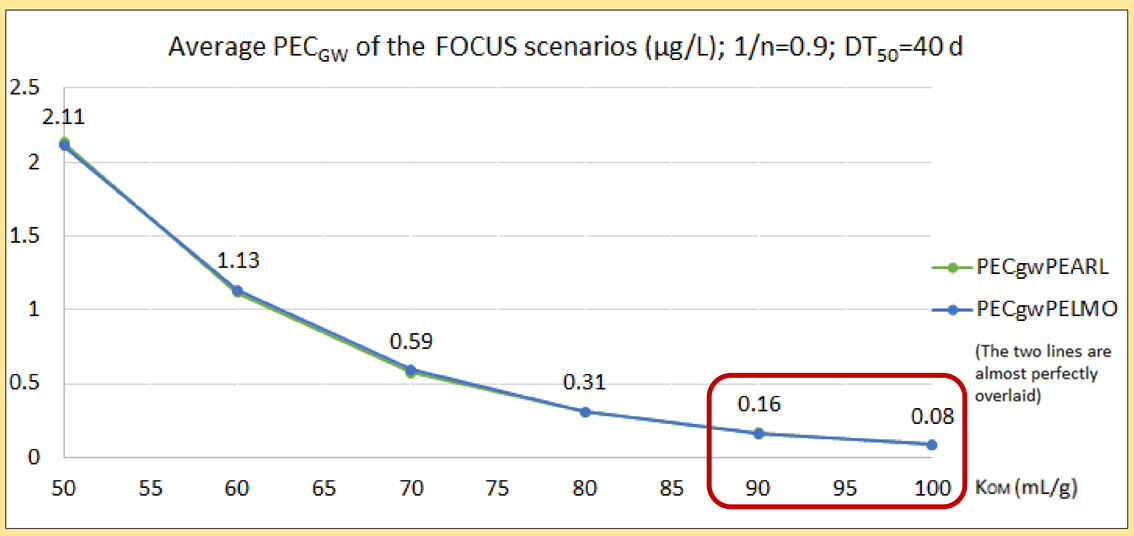
Similar behaviour occurs with higher DT_{50} at higher K_{OM} values.
Scan the QR code at the bottom right for further details.

K_{OM} variation

K_{OM} (mL/g): 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000. DT_{50} (d): 10, 40, 160; 1/n: 0.7, 0.8, 0.9, 1.

Example of significative variations:





Similar behaviour occurs with higher K_{OM} at higher DT_{50} values.
Scan the QR code at the bottom right for further details.

The new input classification sistem approach

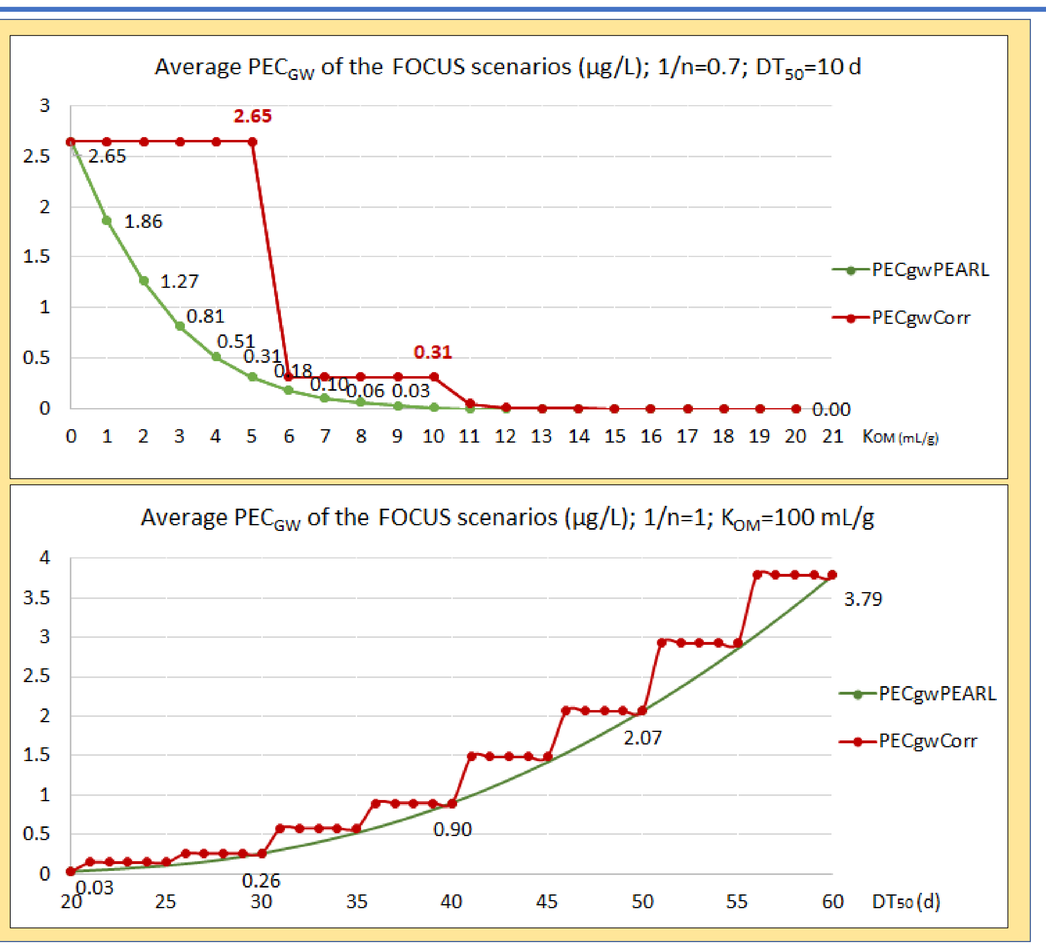
The uncertainty in the K_{OM} determination was assessed by applying the "Horwitz equation" (between-laboratory variability of measurement) to any procedural test result described by OECD Guideline 106.

- A value of about 25% was determined (good agreement with the data on the reference substances reported in the OECD Guideline 121);
- K_{OM} range 0-10 mL/g is a key range for the leaching of substances.

K_{OM} actual (mL/g)	0-5	6-10	>10
K_{OM} corrected (mL/g)	0	5	0.75*K_{OM} actual

Since uncertainties in the DT_{50} determination are more difficult to estimate, a simple interval approach has been adopted.

DT_{50} actual (d)	< 1	0-5	5-10	10-15	15-20	20-25	25-30	30-0	40-50	... +10
DT_{50} corrected (d)	1	5	10	15	20	25	30	40	50	... +10



Conclusions and recommendations

PEC_{GW} models are extremely sensitive to 1/n, K_{OM} and DT_{50}. Significant differences in the results occur also due to input variations smaller than the uncertainty associated to the experimental measures, which is not scientifically sustainable. Some recommendations could therefore be proposed:

It is useless and not scientifically supported to express K_{OM} and DT_{50} using decimals

DT_{50} values <1 d should be considered equal 1 d for modelling purposes

The input classification system proposed above could be used to minimize the effects of the parameters variability

Poster and database: