Uncertainties in groundwater modelling

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The problem

The assessment of the potential **leaching of pesticides in groundwater** is a key point in the registration and authorization process of plant protection products (PPPs) in Europe, under Regulation (EC) 1107/2009. The evaluation is carried out by **FOCUS models**, in particular with PEARL and PELMO models. These models are used to assess the potential movement of crop protection products and their relevant metabolites to groundwater. 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

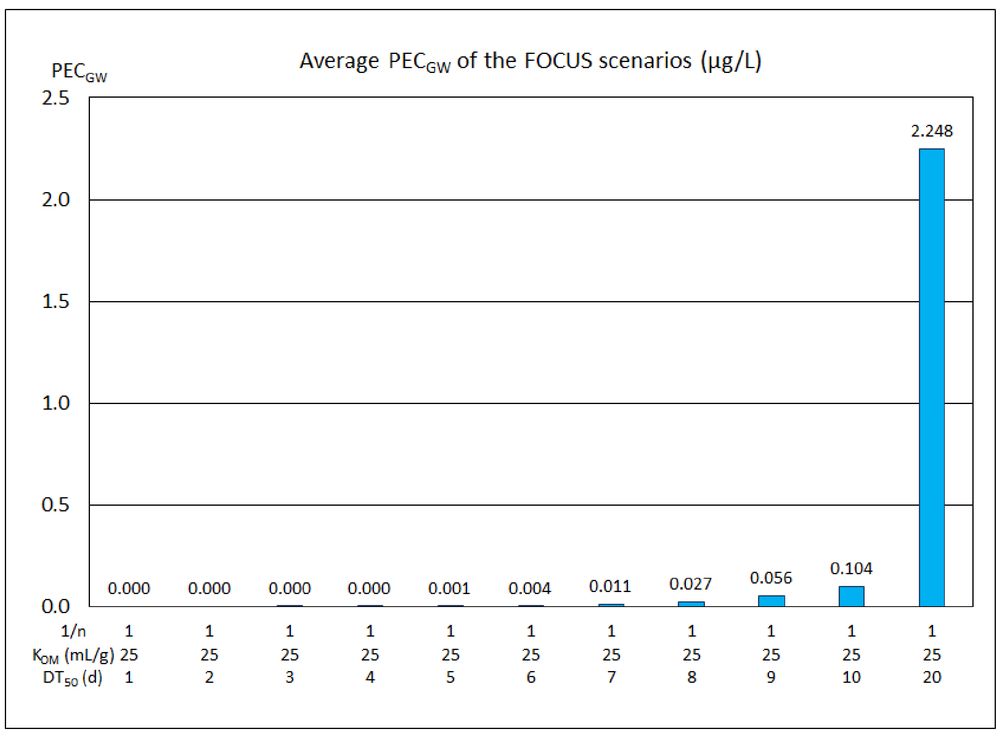
PEC_{GW} calculations have been performed on **808 dummy substances** with various combinations of DT_{50}, K_{OM} and 1/n values, to examine the influence of each single parameter on the final result, and to verify whether the **sensitivity of PEARL model is excessive or not**. Other active substance 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 model 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 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

Substance inputs: 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.

Example of significative variations:



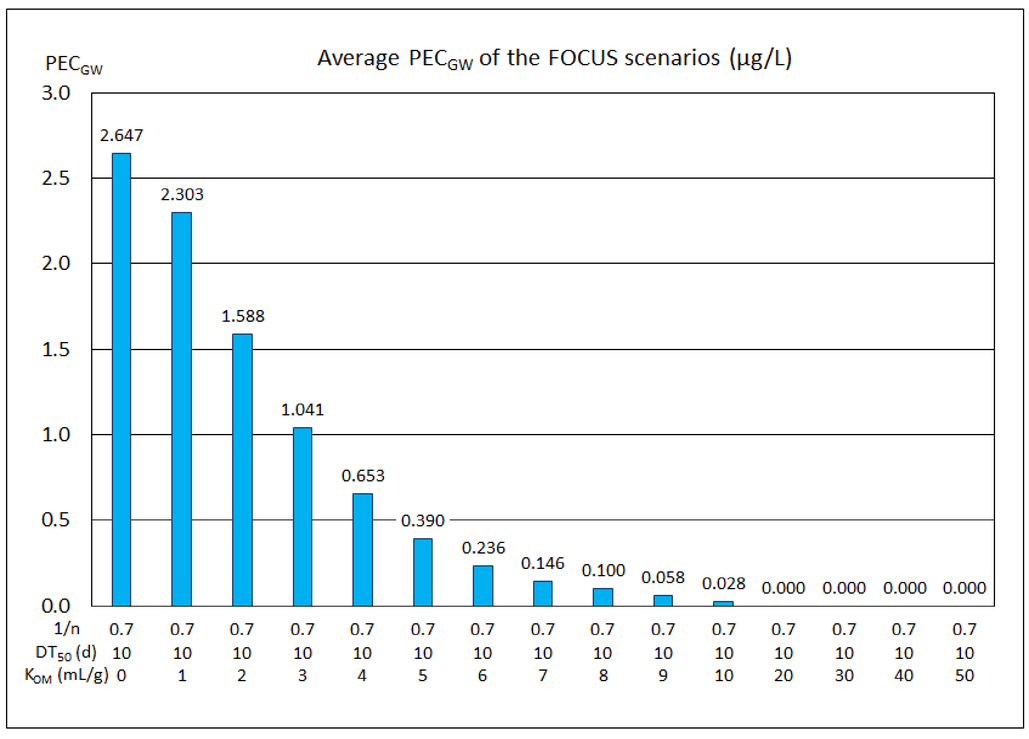
Focus: DT_{50} = 9 d → DT_{50} = 10 d; PEC_{GW} = 0.056 µg/L → PEC_{GW} = 0.104 µg/L

Similar behaviour occurs with higher DT_{50} at higher K_{OM} values. Differences increase for lower 1/n values. See the flyer for further details.

K_{OM} variation

Substance inputs: DT_{50} (d): 10, 40, 160; 1/n: 0.7, 0.8, 0.9, 1;
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.

Example of significative variations:



Focus: K_{OM} = 8 mL/g → K_{OM} = 9mL/g; PEC_{GW}= 0.100 µg/L → PEC_{GW}= 0.058 µg/L

Similar behaviour occurs with higher K_{OM} at higher DT_{50} values. Differences decrease for higher 1/n values, but the sensitivity of the model is too high. See the flyer for further details.

The new input classification sistem approach

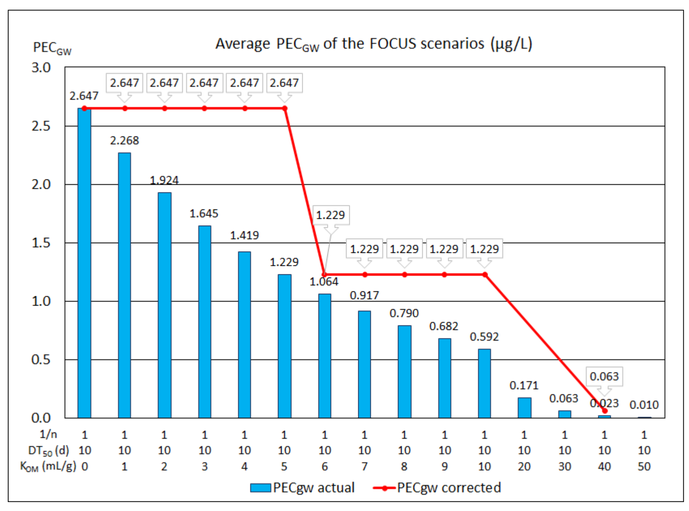
The uncertainty in the K_{OM} determination was assessed by applying the "Horwitz equation" (between-laboratory variability of measurement) to any procedural test result described by OECD Guideline 106. A value of about 25% was determined, which is in good agreement with the data on the reference substances reported in the OECD Guideline 121. In addition, the K_{OM} range 0-10 mL/g is a key range for the leaching of substances.

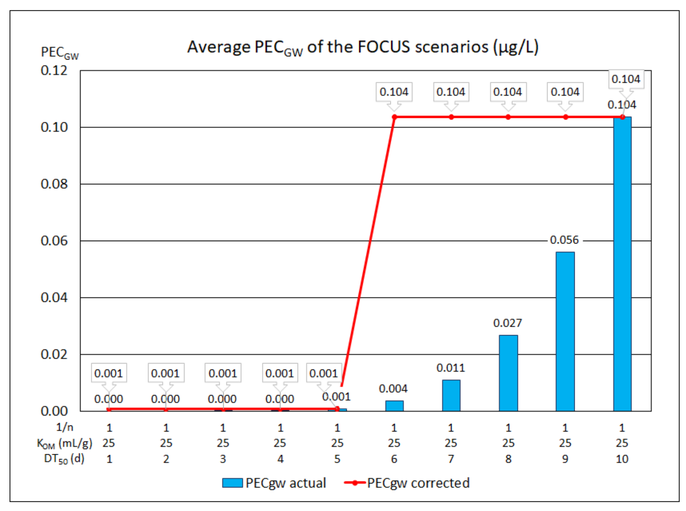
This classification system is therefore proposed:

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 extimate, a simple interval approach has been adopted.
This classification systems was therefore developed:

DT_{50} actual (d)	< 1	0-5	5-10	10-15	15-20	20-25	25-30	30-40	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 model outputs can 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 input parameters K_{OM} and DT_{50} using decimals;
- All DT_{50} values below 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; as a positive side effect, discussion on DT_{50} and K_{OM} determination would reasonably decrease, since slight differences would no more dramatically affect the results.

Feel free to take a flyer if you want to see more graphs. You may ask the authors for the databases produced in this project by e-mail.