METHODOLOGICAL APPROACH FOR EVALUATING FIRST TIER PEC GROUNDWATER SCENARIOS SUPPORTING THE PREDICTION OF ENVIRONMENTAL CONCENTRATIONS OF PESTICIDES AT THE EUROPEAN SCALE

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ABSTRACT
Within the framework of the harmonised registration of plant protection products (PPPs) at the EU-scale, environmental fate models are nowadays combined with a series of scenarios to predict the environmental concentrations of PPPs in the different environmental compartments. At present, harmonised procedures and scenarios for assessing the predicted environmental concentration (PECs) of pesticides in groundwater have been implemented through the FOCUS working groups. The effectiveness and efficiency of the risk assessment procedures will thereby strongly depend on the validity of the environmental fate model and on the validity of the selected scenarios. In contrast to the validation of environmental fate models itself, little attention has been devoted so far to the validation of scenarios.
Within this paper we present a methodological approach for validating scenarios within the framework of risk assessment. The approach was developed within the framework of the EU-FP5 research project APECOP (Effective approaches for predicting environmental concentrations of pesticides) and helps to determine the validation status of the FOCUS groundwater scenarios, as presently used in the higher tier harmonised registration of pesticides at the EU level. Validation encompasses the comparison of PECs to groundwater as obtained using the most detailed modelling approach that currently can be implemented at the Pan-European scale with the results obtained from FOCUS PECs.

KEY WORDS: Pesticide fate modelling, metamodels, validation, scenario evaluation, FOCUS.

INTRODUCTION

For assessing predicted environmental concentrations (PECs) of plant protection products (PPPs) in groundwater, the FOCUS groundwater scenarios working group published nine standard scenarios which, in combination with the FOCUS leaching models, allow to implement a first tier harmonised risk assessment procedure at the Pan-European scale (FOCUS, 2000). Standard scenarios increase the uniformity of the regulatory evaluation process by minimising the influence of the person that performs the PEC groundwater calculation and allow an easier interpretation of the PEC assessment by administrators, regulators and industry (Boesten et al., 2000). The PEC assessment applies to the entire EU, and this implies an appropriate consideration of the variability of soil, crop, climate, hydrology, hydrogeology, agricultural practice, land use and pesticide use within the nine standard scenarios. It is also supposed that realistic worst cases are represented by the standard scenarios. The realistic worst case was identified by the concept that scenarios should correspond to 90^{th} percentile vulnerability situations (FOCUS, 2000). In reality however, the worst case scenario depends on the system properties (weather, soil, groundwater, crop, substance application and chemical properties), which vary considerably in space and time. A correct identification of the worst case scenarios therefore implies the appropriate sampling of the population of a large range of possible scenarios at the EU-level. An estimate of the 90th percentile vulnerable scenario could then be identified from the 90th percentile of the 'unbiased' sample frequency distribution.

Unfortunately, due to limited data availability and limited computing possibilities within an operational registration exercise, a detailed statistical sampling of the population of possible scenarios could not be proposed by FOCUS. Expert judgement was therefore considered to characterize some of the properties of the standard scenarios. Yet, to assure the quality of the PEC assessment, it is of paramount importance to reduce possible bias in such a procedure. In addition, if significant bias would be present in the proposed scenarios, corrections need to be proposed.

In contrast to the number of validation studies for PEC exposure models (see e.g. Vanclooster et al., 2000; Trevisan et al., 2003), little, if any, validation studies for PEC exposure scenarios are presented in the literature. Therefore, no methodological approach is presently available which allows to validate exposure scenarios in a transparent and objective way. The objective of this paper is to present such an approach.

MULTIPLE ASPECTS OF SCENARIO EVALUATION

The FOCUS groundwater scenarios are a set of combinations of soil, crop and climate parameters which in combination with a FOCUS PEC exposure model, allow to assess first tier PECs to groundwater. The PEC assessment takes into account a range of conditions that likely can occur and envisages to evaluate realistic worst cases. Standard scenarios are complex combinations of different land and land use attributes and may therefore be conform to the envisaged use in some aspects, but not in others. The objective of the evaluation of scenarios is therefore to demonstrate the quality of a scenario in its multiple aspects an this in an objective and transparent way. Scenario selection evaluation may result in suggestions to improve the scenario and to reduce the uncertainty in the final assessments.

Given the complexity and the multiple characteristics of a scenario, an "accept or reject" approach is inappropriate. Rather a multi-criterion approach should be pursued allowing to assess the following aspects of the scenario:

1. The *relevancy*, i.e.: Do areas or conditions of PPP use exist for which the scenarios are relevant?
2. The *consistency,* i.e.: Is the definition of the scenario coherent and logic?
3. The *representativity*, i.e.: Is the scenario indeed representative for realistic worst case conditions?
4. The *realism*, i.e.: Do places exist where the soil and climate are well described by the scenarios parameters? Do the scenarios describe existing practices?

For the case of the FOCUS groundwater scenarios, it was considered that the "*realism*" of the scenarios was not an issue. Indeed, scenarios were defined by experts and it is very likely that the conditions of the standard scenario may occur somewhere in Europe. For testing the "*relevancy*", scenario conditions must be coherent with the envisaged use. To illustrate the "relevancy" issue consider the following exemple. Scenarios have been developed as part of the implementation of the 91/414 directive at the EU level. Considering that the conditions of the standard scenarios have been inferred from western European data bases and experiences, the standard scenarios will not be relevant for evaluating PPP emission in the tropical areas of the "Département d'Outre-Mer" of France which also belongs to the EU. This illustrates that the scenarios are irrelevant to some extent. For testing the "*consistency*", it should be analysed if the scenario textual description respect the rules of a reference logic. Semantic techniques such as propositional calculus (Gries and Schneider, 1993) and the extension of the boolean logic to symbolic objects (Bock and Diday, 2000) could be applied to analyse the consistency. Unfortunately, due to time constraints, the "consistency" and "relevancy" aspects of the scenarios could not be evaluated in APECOP. Therefore most attention was paid to the evaluation of the "*representativity"* of scenarios.

Scenarios are defined by their 'intension' (i.e. an ensemble of properties, attributes fully defining the scenario) and are characterised by their 'extension' (i.e. the set of objects corresponding to the properties and attributes defined by the scenarios). The 'intension' of the FOCUS groundwater scenarios can be formalised as follows:

"Places:
(1) inside the major European agricultural areas
AND (2) where realistic worst cases of pesticide leaching occur
AND (3) where the soil and climate have characteristics as defined by a set of chosen parameters.

A worst case of pesticide leaching is equal or greater than the 90th percentile of leaching."

Hence, the FOCUS groundwater scenarios 'intension' has three components: (1) a geographic component (agricultural areas), (2) a statistical component (the 90th percentile of leaching), and (3) a "geophysical" component (soil and climate characteristics).

In order to be operational, 'intension' and 'extension' must be linked by the 'extension function'. In the case of the FOCUS groundwater scenarios, a set of parameters were defined for the reference PEC groundwater models. The PEC groundwater models are the 'extension functions' which allow users to find the required 90th percentile leaching concentrations (i.e. the 'extension') corresponding to the 'intension' of the scenarios.

When evaluating the representativity of a scenario, we compare a 'tested extension' with a 'reference extension'. In other words, we compare the PEC as predicted by means of the PPP FOCUS exposure model (i.e. the 'tested extension') with the ensemble of possible environmental concentrations which may occur in reality, inside major agricultural areas ('reference extension'). The representativity of the worst case scenario is the probability that the worst case PEC predicted by means of the exposure model and the worst case scenarios belongs indeed to the set of real worst cases of environmental concentrations. Hence, to evaluate the representativity, we answer the following question: What is the probability that "FOCUS scenarios are combinations of parameter values selected in such a way that when used in combination with a FOCUS PEC groundwater exposure model, the calculated leaching concentrations are equal or greater than the real 90th percentile of leaching concentrations"?.

To answer this question, it is essential to define the 'reference extension', i.e. the 'real' 90th percentile of leaching concentration. In an ideal world situation, this 90th percentile could be obtained from experimental observations (e.g. detailed monitoring of the presence of PPPs in groundwater). However, our observational skills are presently limited, and therefore the reference 90th percentile cannot be inferred at the European level from empiricism. An alternative is offered by approximating the reference 90th percentile leaching concentration using the most detailed assessment technique that currently is available. Obviously, this type of evaluation has a lower level of security than a validation in which the reference 90th percentile of leaching concentration is estimated from direct measurements. It is expected that through the implementation of the European water framework directive, reference monitoring data will become available and that direct comparison with measurements using techniques such as presented by Worrall (2002) may become possible in the future. However, for the time being, we assign the 90th percentile obtained from detailed spatially distributed exposure modelling to the reference 90th percentile. We therefore compare the 90th percentile of leaching concentration of the 'reference extension' obtained by the 'detailed' assessment technique (further denoted by the superscript *MM*), i.e. $p_{0.9}^{MM}$ with the 90th percentile of leaching concentration with the FOCUS scenario and FOCUS model, i.e. $p_{0.9}^{FOCUS}$. In statistical terms we calculate the probability of the following comparisons: $P(p_{0.9}^{MM} > p_{0.9}^{FOCUS})$, i.e. the probability that the FOCUS scenario is not strict enough or $P(p_{0.9}^{MM} < p_{0.9}^{FOCUS})$, which is the probability that the FOCUS scenario is too strict. In the following paragraphs, we explain how $p_{0.9}^{MM}$ has been calculated.

A HIERARCHICAL SPATIAL SCALE MODELLING APPROACH TO CALCULATE THE REFERENCE LEACHING CONCENTRATION

Leaching to the groundwater is a spatio-temporal process, which is driven by the spatio-temporal variability of site conditions. In the FOCUS procedure, the temporal variability of a leaching event is described by considering long time series (20 years) of daily leaching concentrations as predicted by means of the exposure model using daily meteorological data, and by aggregating the daily leaching concentration to annual values. This is justified by the fact that the within day variability of leaching will be generally (if crack flow is neglected) much smaller than the variability of annual leaching concentration within a period of more than 20 years. This is also justified by the fact that most of the temporal variability will indeed be captured in a time series of 20 years of annual leaching. We therefore assume that the temporal dynamics of a leaching event as generated by the FOCUS procedure corresponds to the temporal dynamics of the 'reference extension'.

In contrast to a detailed description of the temporal dynamics, the spatial dynamics of the leaching event in the FOCUS procedure was only considered by defining worst case soil and climate data for only nine major agricultural areas, referred to as FOCUS areas (FA). The worst case soil data were thereby defined on the basis of expert judgement or previous vulnerability studies carried out at the member state level. Obviously, the within FA spatial variability of the leaching event is thereby not explicitly considered and the effectiveness of the proposed approach will therefore strongly depend on the quality of the expert judgement when selecting the soil and climate data. Recently progress has been made in constructing Pan-European environmental databases such the Soil Profile Analytical Database (SPADE), the climate database (MARS). Therefore, given the availability of detailed soil map information at the Pan-European level, a detailed spatially distributed and explicit statistical based approach could be proposed for estimating the 90th percentile of leaching concentration of the 'reference extension'. An explicit spatially distributed approach allows to capture the spatial variability of the leaching event in detail and reduces thereby the subjectivity in defining worst case soil types. Additionally, the expert judgement (FOCUS, 2000) was based on the assumption that an overall 90th percentile leaching is attained when the vulnerability is separated in two supposed independent components: vulnerability of soils (spatial component) and climate (time component). The procedure was said to be equivalent to take the 80^{th} percentile of leaching from the time series, and the 80^{th} from the remaining spatial component of the variability. It can be easily demonstrated that such an assumption is not statistically funded. This, however, does not invalidates the scenarios since the real expert judgement can lead to a 90^{th} percentile vulnerability even if its theoretical justification is false. In any case, the methodology we present avoids such a problem.

The estimation of the 90^{th} percentile of leaching concentration of the 'reference extension' is made by means of detailed numerical analysis where detailed Pan-European spatially distributed soil, climate and agricultural data were processed. For the spatial schematisation of the leaching event, three hierarchical spatial levels were considered (Figure 1):

1. the point scale level for which a point scale leaching concentration (PS_PEC) is calculated;
2. the grid scale level, corresponding to a regular grid of 10 x 10 km^2, for which a grid scale leaching concentration (GS_PEC) is calculated;
3. the regional scale level (the FOCUS area or Europe), for which the regional scale leaching concentration (RS_PEC) is calculated.

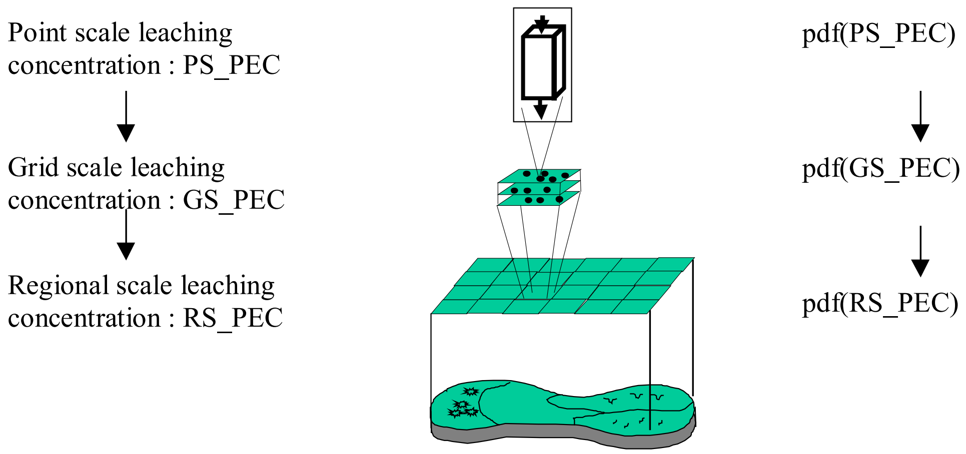

Figure 1: The multi-scale spatially distributed exposure modelling approach.

At each spatial level, the leaching concentration is fully characterized by a probability density function (pdf), which allows to infer the required percentile. The local scale pdf of the leaching concentration reflects the uncertainty related to i) the use of the point scale exposure model, ii) the use of effective point scale model parameters thereby ignoring pore scale variability; and iii) the temporal variability of the annual leaching concentration. The grid scale pdf further considers the variability of the soil parameters within a 10 x 10 km^2 grid. The regional scale pdf finally encodes the variability of the grid scale parameters within the region. The upscaling from the point scale to the grid scale is done by considering that the grid scale is a mixed distribution (Bishop, 1995) from each individual point scale pdf. In the same way, the regional scale pdf is a mixed distribution of the grid scale pdfs.

META-MODEL APPROACHES FOR EXPOSURE MODELLING

The conceptually based, spatially distributed numerical model as described by Tiktak et al. (2003ab) (i.e. the EuroPEARL model) suffers from some limitations. First the conceptually based modelling approach makes the calculation of the model for a large set of soil, crop and climate parameters a computer intensive exercise. Second, the modelling procedure can presently only be implemented for 75 % of the European agricultural area, since no soil data are available in the SPADE soil profile analytical data base for 25 % of the agricultural area. Finally, the model ignores the variability of soil properties within the Soil Mapping Units (SMUs) by using only the dominant Soil Typological Unit (STU) within each SMU. To avoid these limitations, a meta-model was derived from the EuroPEARL model. The meta-model relates the annual leaching concentration at 1 m depth (the FOCUS target depth) as calculated by means of EuroPEARL to a set of basic soil and climatic input parameters. The mapping of the EuroPEARL results into the meta-model is realised by means of radial basis artificial neural networks. Input parameters for the meta-model were long term average mean seasonal climatic data (rain and temperature), the top- and subsoil available water, organic matter, sand and clay content, and packing density.

In contrary to other regression methods, artificial neural networks outperform in terms of flexibility and versatility. Radial basis neural networks are described in detail in Bishop (1995). The outputs of the neural network are simply the summation of a number of functions (called basis functions, ϕ) multiplied by weights w:

$$y(\mathbf{x}) = \sum_{j=1}^{t} (w_j \Phi_j(\mathbf{x})) + w_0$$

where y is the output vector of the neural networks (i.e. log transformed mean and standard deviation of the annual leaching concentration, which after inverse transformation allows to calculate the $p_{0.9}^{MM}$); w_j are the weights; x is the input vector to the neural network (i.e. e.g. the long term mean spring precipitation or the percentage of organic carbon, etc…); and Φ the basis functions, represented by Gaussians:

$$\Phi_j(\mathbf{x}) = \exp\left(-\frac{\left\|\mathbf{x}-\boldsymbol{\mu}_j\right\|^2}{2\boldsymbol{\sigma}_j^2}\right)$$

where μ_j and σ_j are the parameters of the basis functions. During the network training (i.e. the meta-model calibration), the vectors μ**,** σ and $\mathbf{w}$ are determined using the outputs of the EuroPEARL model and the meta-model input. μ_j are determined by fitting a Gaussian mixture model with circular covariances, using the EM algorithm (expectation-maximization, Dempster et al, 1977; Bishop, 1995); σ is set to the maximum inter-centre squared distance and the w_j that give rise to the least squares solution can be determined using the pseudo-inverse (Nabney, 2001).

IMPLEMENTING THE EVALUATION OF THE REPRESENTATIVITY OF THE SCENARIOS

The reference 90th percentile leaching concentration in each FOCUS area is characterised as follows. First, the annual leaching concentration at 1 m depth is calculated with the EuroPEARL model (Tiktak et al., 2003ab). Then, a metamodel is constructed to predict the reference 90th

percentile leaching concentration for all the plots in the area. Sofar, the evaluation of the representativity of the scenarios was only tested for one single pesticide (pesticide D in the FOCUS scenario report), and considering two major agricultural crops (maize and winter wheat). This implies that the vulnerability is considered to be driven mainly by the vulnerability of soil and climate, not by vulnerability of crops which corresponds to the definitions of the FOCUS scenarios (see FOCUS, 2000).

Metamodel parameters

The selection of the metamodel input parameters depends on the availability of Pan-European soil and climate maps, or on the existence of reliable pedotransfer functions. The following parameters were selected:

- soil packing density (top/subsoil)
- soil available water (top/subsoil)
- texture (top/subsoil sand, top/subsoil clay)
- organic matter content (top/sub soil)
- rainfall (long term average, year, spring, autumn)
- air temperature (long term year average)

Soil data preprocessing

For implementing the meta-model, use was made of the European soil map at the scale of 1:1000.000 (CEC, 1985) and the associated soil geographical data base (King et al., 1994). The soil map is characterized by Soil Mapping Units (SMUs). The associated database contains a table that defines the percentage in area of a given Soil Typological Unit (STU) in the SMU. Another table defines for each STU the top soil properties. Like in the SPADE data base (Madsen-Breuring and Jones, 1995), which was used for the EuroPEARL parameterisation, these properties have been defined on the basis of expert judgement. In contrast to SPADE, it contains only class data, and generally only data for the top soil. Therefore, data from the soil geographical data base were preprocessed to generate the continuous basic top and subsoil data which are needed as input to the metamodel for each STU. In order to give numerical values to the classes, a mean value for each class was calculated and chosen as representative for the class. Additionally, use was made of the meta data pedotransfer functions (PTF) rules as presented by Daroussin and King (1996). Due to lack of data, subsoil organic matter content was set equal to zero which corresponds to the most critical situation from a leaching point of view. Subsoil texture has been calculated from the topsoil texture using pedotransfer functions derived from SPADE. Using this approach, basic soil data could be defined for 97 % of the total area. The quality of the data generated was checked by comparing the mean and variance of the data of the considered properties as used in EuroPEARL and inferred from SPADE with the data generated through this approach. Tests were acceptable, except for the packing density for which a scaling procedure was implemented.

Calibration of a meta-model

Ninety percent of the EuroPEARL simulations were used for the calibration of the meta-model, while 10 % were used for validating the meta-model. Prediction of the error of the meta-model in terms of the leaching concentrations predicted by the EuroPEARL model is illustrated in the Fig. 2.

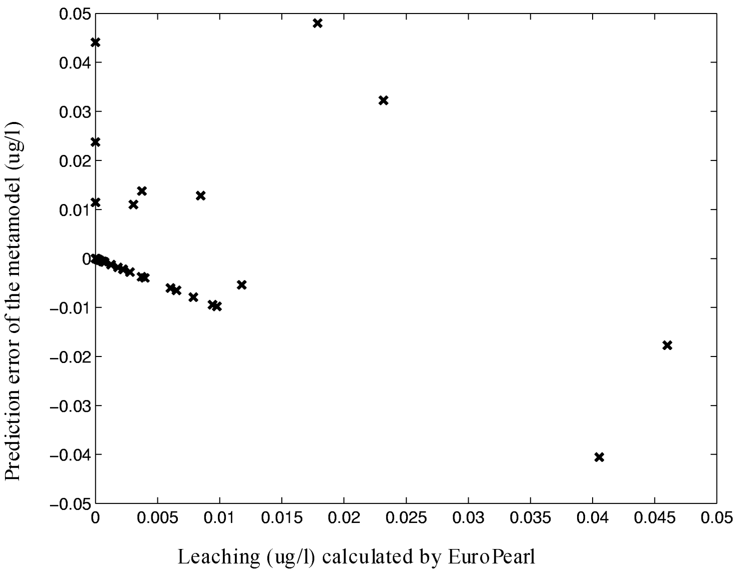

Figure 2. Prediction error of the metamodel in terms of the calculated leaching concentration with the EuroPEARL model for the validation data set

Modelling efficiency of the meta-model equals 0.89 for the predicted mean annual leaching concentration and 0.66 for the predicted annual standard deviation. The median of the error in absolute terms equals 0.0145 µg/l for the predicted annual mean, and 0.0187 µg/l for the predicted annual variance. Given that the prediction error is situated in the same order of magnitude of the EuroPEARL simulation, it was considered that the meta-model was appropriate for evaluating the representativity of the scenarios.

Calculation of European leaching maps

Next, maps of the 90^{th} percentile of leaching concentration were generated using the hierarchical spatial schematisation presented above:

- The point scale pdf, pdf(PS_PEC)), was calculated for each STU by means of the above mentioned meta-model.
- The grid scale mixed pdf of the leaching concentration, pdf(GS_PEC), was calculated numerically from the point scale leaching concentration pdf's. The point scale pdf's were weighed by percentage coverage of a STU within a grid to yield the grid scale pdf. For such a purpose, the percentage coverage of a STU inside a cell was considered equal to its coverage in the SMU where the cell is located.
- The grid scale pdf's are used in a last step to generate the grid map of the 90^{th} percentile of leaching concentration over Europe (i.e. the 90^{th} percentile is calculated for each grid cell using the corresponding pdf(GS_PEC)).

An example of a leaching map for substance D is given in the figure 3.

Performing the evaluation test

In a final step, the generated regional scale leaching concentration pdf (pdf(RS_PEC)) is generated from the grid scale pdf (i.e pdf(GS_PEC) and can be used to perform the representativity evaluation test. For such a purpose, $p_{0.9}^{MM}$ - for the whole Europe and for each Focus Area - is estimated from pdf(RS_PEC). Then, $p_{0.9}^{MM}$ is compared to $p_{0.9}^{FOCUS}$ in a probabilistic way as explained before. $P(p_{0.9}^{MM} > p_{0.9}^{FOCUS})$ is calculated from pdf(RS_PEC) using a Monte-Carlo approach which allows to take into account uncertainties coming from the soil and climate maps, as well as from the numerical and meta-models. Such tests allow to evaluate the representativity of a scenario for a given substance in a statistical verifiable way. The test can be performed both at the European scale (considering that the scenarios are representative for a global 90th percentile), or for each Focus Area (considering instead that a given scenario is representative for its corresponding area).

Figure 3: 90th percentile leaching concentration for substance D and winter wheat, as calculated by means of the hierarchical spatial parameterisation scheme and the artificial neural network meta-model.

CONCLUSIONS

In this paper, a methodological approach is presented for evaluating the FOCUS groundwater scenarios. A multi-criterion approach is proposed considering the multiple aspects of scenario evaluation, i.e. the test of the 'relevancy', the 'realism', the 'consistency' and the 'representativity' aspects of a scenario.

Details are given for the 'representativity' aspect of scenario evaluation. Results from FOCUS calculations are suggested to be compared to the results from a fully spatially distributed exposure modelling approach. The spatially distributed modelling approach allows to calculate in a statistically verifiable way, the percentiles of leaching concentrations in terms of spatially variable land attributes (soil and climate). Full coverage of the European territory is thereby obtained by combining the simulation of a conceptually based numerical model (the EuroPEARL model) with an artificial neural network based meta-model. In the presented methodology, the meta-model and the numerical model are complementary and remains mutually dependent since the meta-model is calibrated on data generated by means of the numerical model. At the same time, the meta-model can be applied in situations where one is confronted with data scarcity or when Monte-Carlo analysis is expected to be performed to propagate uncertainty in the PEC estimate. These advantages compensate for the additional error introduced by the use of a meta-model in stead of the detailed numerical model. The data generated through the hierarchical spatially distributed modelling approach can now be used to assess the representativity of a scenario in a statistical sense.

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