Comparison of pesticide leaching potential to groundwater under EU FOCUS and site specific conditions

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Abstract

The EU FOCUS scenarios are a set of nine standard scenarios based on a combination of crop, soil and weather data used throughout Europe to evaluate the leaching potential of pesticides to groundwater. In Ireland, two predefined EU FOCUS scenarios (Oakehampton and Hamburg) appear to be the most appropriate to Irish conditions. However, there is concern that these scenarios may not accurately represent Irish specific conditions, especially in terms of soil and climatic weather. Therefore, the objective of this study was to parameterise a number of site specific locations in Ireland (represented by Oakpark, Clonroche, Rathangan and Elton series soils) and to compare simulated leachate levels at these locations to EU FOCUS scenarios using the PELMO ("Pesticide Leaching Model") simulation model. The hydrological processes were validated using observed data for soil tension and leachate. The appropriate EU FOCUS scenarios were then simulated for the given locations and compared to the parameterised scenario. All scenarios were run using the same version of PELMO, therefore eliminating any software impacts. The models were run for 26 years using appropriate meteorological data. The results showed significant difference between the parameterised model pesticide leaching and that resulting from the EU FOCUS scenarios, the latter overestimating site pesticide leaching from 42 to 99%. The results indicated a significant conservatism in using EU FOCUS scenarios to determine potential pesticide concentration in the leachate under Irish specific conditions and ensure the desired level of protection against pesticide contamination of national water resources.

Key words: Pesticide; PELMO; EU FOCUS groundwater scenarios; Leaching potential.

1. Introduction

Pesticides are chemicals used in a wide range of areas (e.g., agriculture, forestry and urban amenity) to control pests (e.g., weeds, birds, insects and viruses) (CEC, 2007). In crop production, pesticides may be used to improve crop yield, which may in return result in the improvement of food availability (Cooper and Dobson, 2007). Despite their important role, the use of pesticides can have negative effects on non-target organisms, water and soil compartments, while also potentially impacting human health (Pavlis et al., 2010). The negative influence of pesticide on water quality and biota has been reported (Andreu and Picó 2012; Blasco and Picó 2009). A coordinated effort at global and regional level on the use of pesticides is needed to ensure crop protection with the view to ensuring food safety and quality while protecting the environment (Carvalho, 2006).

Several ranking tools have been developed to give a quick evaluation of the potential risks associated with pesticide use on agricultural land and various techniques are available including scoring approaches, decision trees and risk ratio methods (Labite et al., 2011; Wustenberghs et al., 2012). At the European level, Directive 91/414/EEC stipulates that before EU countries licence plant protection products, associated risks (e.g., risk to human health, including workers, soil contamination, air, surface and groundwater contamination) must be evaluated (CEC, 1994). The recommended approach is based on the ratio of the predicted environmental concentration and the appropriate toxicological data for air, sediment, soil, surface water and groundwater (CEC, 1994). For groundwater, the FOCUS (i.e., Forum for the Coordination of Pesticide Fate Models and their Use) groundwater workgroup was set up to develop a set of standard scenarios that can be used to assess the leaching potential of pesticide to groundwater (FOCUS, 2000; FOCUS, 2009). In FOCUS groundwater, nine scenarios, (based on data from Châteaudun located in France, Hamburg in Germany, Jokioinen in Sweden, Kremsmünster in Austria, Okehampton in United Kingdom, Piacenza in Italy, Porto in Portugal, Sevilla in Spain and Thiva in Greece) have been developed based on a combination of crop, soil and weather data for these sites. In addition to these scenarios, four environmental fate models, PEARL, PRZM, PELMO and MACRO were selected within the FOCUS groundwater framework. In the first release of the FOCUS groundwater models, all models, except MACRO were based on the convection dispersion process (i.e., chromatographic flow) in soils and parameterised for all the nine scenarios. MACRO, which is a preferential flow model, was only parameterised for the Châteaudun scenario. In a preferential flow process (in contrast to the chromatographic flow), it is assumed that water and chemical transport occurs with by-pass in macro pores, and this can introduce a bias in the risk assessment if the process is not considered. To date, efforts are being made to include the process of preferential flow in all FOCUS environmental fate models, although this is at a preliminary stage (FOCUS, 2009). Most EU countries refer either to one or more of these scenarios when assessing the leaching potential of pesticides. Some countries (e.g. France and Sweden) have elaborated their own scenarios to reflect the agro environmental conditions of their countries (FROGS, 2011; FOCUS, 2009). In Ireland, the registration of Plant Protection Products is based on using the Okehampton and Hamburg scenarios with PELMO, as these scenarios are most appropriate for Irish conditions, but have limitations, including the relevance to Ireland of soil and weather conditions used in the scenarios (Zhang and Moody, 2004). Recently, the work of Piwowarczyk (2013), who studied pesticide adsorption parameters in soils for several locations, generated site sorption data which can be used to model and predict the leaching potential of pesticides to groundwater. The objective of this study is to parameterise and validate leachate flow from a number of Irish specific locations using the PELMO pesticide leaching modelling tool and compare pesticide concentration predictions from the EU FOCUS scenarios applied to the same sites.

2. PELMO description

The PELMO model is a one dimensional model which simulates water and chemical movement in the unsaturated zone within and below the plant root zone (Ferrari et al., 2005; Klein et al., 1997). It simulates soil hydrology based on a “tipping bucket approach” where water will move to the next layer if the field capacity is exceeded while solute transport is based on convection-dispersion process (Klein et al., 1997; FOCUS, 2000). The PELMO model has been tested by the model developers (Klein et al., 1997; Klein et al., 2000) as well as third parties (Boesten, 2004; Dubus et al., 2003; Ferrari et al., 2003) to predict the environmental concentration of pesticides. The main processes in the model include water movement, chemical transport, substance degradation, sorption, volatilization, run off, soil erosion, soil temperature, plant uptake and substance application (FOCUS, 2009). Klein et al. (1997) noticed that predicted water flow and pesticide transport were of the same order of magnitude. The wide range of inputs (including soil, climate and pesticide parameters) and their importance in PELMO have been evaluated by Klein et al. (2000) and Dubus et al. (2003). Based on the lessons learned from previous versions, the 4.4.3 version of the model was developed to improve the model predictions. In the 4.4.3 version of PELMO (which is more user friendly), the volatilisation (from soil surface and plants) and sorption of pesticide to soil processes have been upgraded and the preferential flow module has been included (FOCUS 2011). Volatilisation from the soil surface was assumed to be temperature dependant in the 4.4.3 version in contrast to the previous versions. In addition, the plant volatilisation was refined by considering volatilisation from leaves and photodegradation. With regard to pesticide sorption to soil, the pH dependency and kinetic sorption modules were made available if necessary to improve the sorption process description. Recently, the concept of preferential flow has been included in the PELMO model using three parameters: threshold daily rainfall, fraction of excess rainfall, and macro pore depth (FOCUS, 2009). The process of macropore flow in PELMO is activated when the threshold rainfall value is exceeded where a certain proportion of rainfall (i.e., fraction of the excess rainfall) will be routed into macro pores at a fixed depth. For this study, the simulations were performed with the latest version of PELMO (i.e., version 4.4.3).

3. Modelling strategies

The overall modelling approach used in this study for assessing the risk of pesticide leaching is detailed in **Fig. 1.** A wide range of inputs were required (soil data, meteorological conditions, pesticide properties and management practices) and were grouped into three categories: site, climate and pesticide input parameters (FOCUS, 2000; FOCUS, 2009). The overall strategy adopted was to parameterise the site specific scenarios in PELMO, calibrate the hydrology for the selected sites followed by pesticide simulation for the sites. The simulation results were then compared to the EU FOCUS predictions (*viz* Hamburg and Okehampton scenarios). The hydrology was calibrated by comparing the predicted quantity of percolation water to observed water percolated and soil tension data. Firstly, the observed water percolation data were obtained by regular measurements from undisturbed lysimeters containing four Irish grassland soils (i.e., Oak Park, Clonroche, Rathangan and Elton soil series). The experiments were carried out at Teagasc Johnstown Castle Environmental Research Center from 3/8/2006 to 24/3/2008 and are detailed in Kramers et al. (2012). Secondly, the soil tension measurements were conducted at Oak Park Research Centre, Co. Carlow, at well drained sites under cereal production. The soil tension measurements were recorded at 0.3 and 0.6 m depth and the details of the experimental conditions were described in Premrov et al. (2010).

3.1. Site description

Based on diversity of soil, location and data availability, four locations were selected for simulation: Oak Park (County Carlow), Clonroche (County Wexford), Rathangan (County Wexford) and Elton (County Limerick). The soils selected have contrasting textures throughout their horizons with their key characteristics presented in Table 1. The depth of the soils is variable and a previous study highlighted differences in preferential flow as a result of earthworm activity in these soils (Kramers et al., 2012). Preferential flow through deep earthworm burrows was observed in the Clonroche, Elton and in particular in the Rathangan soil (burrows down to 1 m depth). Preferential flow in the Oakpark soil is likely to be a combination of shallow earthworm burrows and unstable infiltration in this coarse-grained soil (Kramers et al., 2012). The predominant land uses for the Oakpark and Clonroche soils is tillage and grassland for the Rathangan and Elton soils.

3.2. Simulation with PELMO

For each scenario, the model was parameterised using site specific soil and climatic data while the pesticide parameters used were common for all scenarios (EU FOCUS scenarios and site specific scenarios).

3.2.1 Soil and climatic input data

- *EU FOCUS scenarios*

The Okehampton and Hamburg scenarios were parameterised in PELMO using FOCUS data. A number of climate parameters are required as inputs in PELMO: daily rainfall, evapotranspiration, daily temperature at 2 pm, daily mean temperature, daily temperature difference and annual average relative humidity. A total of 26 years weather data for Okehampton and Hamburg was set up in the FOCUS scenarios and used for the Oakhampton and Hamburg scenarios (FOCUS, 2011).

- *Site-specific scenarios*

Similarly to the FOCUS Okehampton and Hamburg scenarios, daily rainfall, evapotranspiration, daily temperature at 2 pm, daily mean temperature, daily temperature difference and annual average relative humidity for a total of 26 years weather data of Kilkenny and Oak Park weather stations were used for the Oak Park scenario. Rosslare and Johnstown weather stations data were used to model Clonroche and Rathangan scenarios and for the Elton scenario, Shannon Airport weather station data were used (Met Éireann, 2013).

The model was parameterised using the physical soil properties (i.e., pH, bulk density, organic carbon, sand, silt and clay content) of Oak Park, Clonroche, Rathangan and Elton soils **(Table 1)**. Soil field capacity can be calculated from the internal pedotransfer function of PELMO based on the sand and clay content (Klein, 2000). The value of 30% suggested by Kramers (2009) was used for initial soil water content for all the sites. In the FOCUS groundwater framework, the results of pesticide leaching to groundwater are reported at a minimum depth of 1 m. Where soil properties were not available for deep layers, values of the layer above were repeated, consistent with standard approaches (FOCUS, 2000).

The simulations in PELMO require crop input parameters and this includes emergence, maturity, senescence and harvest date, and root depth. Grassland was selected due to its importance in Ireland as it accounted for more than 90% of the total area and received more than 82% of the weight of active substances applied (DAFF, 2003); spring cereals were chosen to model a tillage scenario. Due to limited studies of Irish crop specific parameters (e.g., root depth, crop interception and fate of pesticide on plant surface), the Okehampton crop parameters set up in FOCUS were selected to model Irish sites and a default value of 0.5 was used to model plant uptake (FOCUS 2000). In addition to soil properties, the scenario file in PELMO requires a degradation factor and pesticide dispersion properties to characterize pesticide fate in the environment. The former is included in PELMO to take into account the influence of microbial activity in combination with soil type on pesticide degradation. In the absence of Irish site specific degradation parameters and due to the limited data available to account for the depth dependency factor, 1, 0.5, 0.3, and 0.3 were used for all soils and depths. In PELMO, a realistic description of the pesticide dispersion process in soil can be simulated with dispersion depth values varying from 2.5 to 5 cm (FOCUS, 2009). For the dispersion depth, the default values of the thickness of soil compartments and dispersion length of 2.5 and 5 cm (model default) were used by assuming constant dispersion in the entire soil profile. Free drainage was assumed for all scenarios and additional default values for the simulations were detailed in the supplementary material.

After initialization, site input parameter sensitivity was analyzed by changing each by ± 10 % of their initial values while keeping all other parameters constant. In addition, the thickness of soil layers (i.e., calculation unit) was set at 5 cm, recognizing its importance in influencing pesticide dispersion (FOCUS, 2000; FOCUS, 2009). Moreover, preferential flow in PELMO was simulated due to its occurrence in the unsaturated zone and this can potentially increase dramatically the risk of pesticide leaching to groundwater, as highlighted in several studies (Kördel and Klein, 2006; Scorza Júnior et al., 2007; Vanclooster et al., 2003). The only published study on the use of preferential flow in PELMO was Jarvis et al. (2003) who conducted preliminary tests of the preferential process in PELMO for two clay soils Lanna and Andelst. To model the preferential flow in these soils by using PELMO, the following inputs were specified: macropore depth, daily rainfall, and fraction of the excess were set to 70 cm, 5 mm and 0.5, respectively for Lanna sites and to 85 cm, 10 mm and 0.25, respectively for the Andelst site. In this study a default value of 50 cm, 2 mm and 0.3 were used for the macropore depth, threshold daily rainfall and fraction of the excess rainfall, respectively to parameterise macropore flow in PELMO.

3.2.2 Pesticide selection and input parameters

Three commonly used pesticides MCPA, Mecoprop-P and Chlorothalonil used in the Irish agricultural sector were selected and due to the availability of adsorption data for those chemicals (Piwowarczyk, 2013). Out of 85 pesticides surveyed at national level, MCPA, Mecoprop-P and Chlorothalonil represented 40.87, 13.74 and 1.27 %, respectively, of the total active substances used for grassland treatment based on the weight (DAFF, 2003). In addition, the work of Labite and Cummins (2012) highlighted the first two compounds (i.e., MCPA and Mecoprop-P) as potential chemicals of human health concern. The sorption, degradation and volatilisation parameters used in the model are described in **Table 2, 3** and in the supplementary material. The pesticides were assumed to be applied twice on grassland (April 15th and July 15th) and once for tillage soils (May 1st) at the application rate described in **Table 3** for every year over a period of 26 years. These application doses correspond to the recommended values by the

Pesticide Control Service for Grass and spring cereals (Personal communication, Irish Pesticide Control Service 2012). To allow comparison of each pair of site specific scenarios and the Okehampton and Hamburg scenarios, the crop, pesticide parameters, management and application rates were kept the same for each scenario so that the differences were due to the soil and weather parameters only.

3.2.3 Model efficiency

Model efficiency (EF) was assessed **(Eq. 1)** for PELMO with site specific parameterisation and the same indicator used to assess sensitivity to input parameter choice: where O_i is the observed percolate (in mm); Ō the mean observed value (in mm); Pi the predicted percolate (in mm). The maximum EF value of 1 indicates that the predicted and observed values are equal and the model is perfect and a value less than -1 is regarded as unacceptably poor, i.e., the model prediction should not be used for predictive purposes (Vanclooster et al., 2003; Loague and Green, 1991; Walker et al., 1995).

$$EF = \frac{(\sum_{1}^{N}\left(O_i - \overline{O}\right)^2 - \sum_{1}^{N}(P_i - O_i)^2)}{\sum_{1}^{N}\left(O_i - \overline{O}\right)^2} \qquad \textbf{(1)}$$

4. Results and discussion

4.1. Model efficiency, sensitivity and calibration

The model efficiency, sensitivity and calibration results for Oak Park were presented in **Table 4**. After parameterisation of the PELMO model, an EF value of -1.96, indicating unacceptable prediction was achieved **(Table 4)**. Following sensitivity analysis the best EF was obtained by increasing the soil compartment depth from 2.5 to 5 cm and then the change by ± 10% of the root depth initial value by adjusting root depth. Each soil layer was therefore adjusted to 5 cm to achieve the best prediction of leachate, which was, also consistent with the work of Akbar and Akbar (2012) who found that soil horizon (and layer) thickness was the most important input parameter.

Following the calibration, PELMO, was validated using lysimeter data conducted from Johnstown Castle (Kramers et al., 2012) and field observations Oak Park (Premrov et al., 2010), respectively. The predicted and observed cumulative daily percolate for Oak Park, Clonroche, Rathangan and Elton are presented in **Fig. 2**. PELMO was able to predict the total amount of percolation water for the sites although the model slightly underestimated water percolated for Rathangan and Elton soils.

The lowest level of water percolation was noticed in Rathangan soil for both, i.e., the experimental observations and the predictions. One of the reasons may be due to its high clay content (ranging 19 to 29%), especially in its deeper horizons. According to Brown et al. (1995) and Carter (2000), clay soils contain less coarse pores (in contrast to sandy soil) which are responsible for the slow water movement. The observed low percolation might also due to the presence of dead end pores at the site as a low recovery of tracer was observed on this soil type (Kramers et al., 2012). The percolation simulated for all soils showed a plateau in 2007 for all the sites and the probable explanation could be due to the dry conditions which occurred in the year 2007 with the annual rainfall of 754 mm for Rathangan and Clonroche, 844 mm for Oak Park and for Elton 922 mm (with the average annual long term rainfall of 912, 842 and 982 mm, respectively). The mean annual temperature in 2007 for Rathangan and Clonroche was 12.64 °C, for Oak Park 10.5 °C and for Elton 11.1 °C (with the average annual long term temperature of 10.9, 9.6 and 10.6 °C, respectively).

The results **(Fig. 3)** showed an inverse relationship between the predicted percolate and observed soil tension at 0.3 and 0.6 m depth. The peak values of the model predictions highlighted the potential occurrence of the leaching events. This confirms the model's ability to capture hydrological processes.

4.2. Pesticide simulation: EU FOCUS versus Irish site specific scenarios

The 26 year simulation representing the site specific scenarios and FOCUS Okehampton and Hamburg scenarios, are presented in **Table 5**. The results showed that more chemical was predicted to leach with the FOCUS Okehampton and Hamburg scenarios simulations compared to the site specific scenarios **(Table 5)**. The simulated leaching potential of pesticide using the Okehampton and Hamburg scenarios differed to that compared to the simulated Irish conditions with a difference ranging from 42% (Rathangan grass versus Hamburg grass scenarios) to 99.6% (Clonroche grass versus Okehampton grass and Oak Park tillage versus Okehampton tillage). The use of standard scenarios may not appropriately allow the evaluation of the leaching potential of pesticides to groundwater as the environmental conditions (i.e., rainfall, temperature and soil conditions) are highly variable at local or regional level (van Alphen and Stoorvogel, 2002). In Sweden for example, the national registration authorities of plant protection products identified the most vulnerable areas based on the combination of Swedish hydro-geological conditions, weather data and major crop types and use of pesticides in Swedish agriculture. A comparison of the Swedish scenarios to the EU FOCUS Scenario Châteaudun (which is the only EU focus scenarios applied to the Swedish situation) revealed that the FOCUS Châteaudun scenario underestimated the leaching potential of pesticides to groundwater for all the Swedish scenarios (Jarvis et al., 2003 and KEMI, 2010). This highlights the importance of comparing the EU FOCUS groundwater scenarios to site specific conditions, and several European countries (e.g., France, Sweden, Czech Republic and Sweden) have defined their own scenarios which allow the protection of vulnerable areas (FOCUS, 2009). However to date, several European countries use one or more of the predefined EU FOCUS groundwater scenarios to assess the leaching potential of pesticides to groundwater as their national procedure for pesticide registration (FOCUS, 2009).

In this study, the difference of the Okehampton and Hamburg scenarios to Irish scenarios may be explained due to the soil and climatic conditions. A comparison of organic carbon, clay, silt and sand content and climatic conditions at the different sites is shown in **Fig. 4 and 5**. The evaluation of the soils and climatic conditions revealed heterogeneous composition of organic carbon, clay, silt and sand content throughout the profile of all scenarios. The Okehampton and Hamburg scenarios were characterised by having less organic carbon than the Irish scenarios, except in one occasion where the amount of organic carbon in the B horizon of the Hamburg scenario is higher than the one of Rathangan **(Fig. 4)**. Among the Irish scenarios, Rathangan exhibited the highest pesticide leaching potential and Clonroche the lowest based on the highest and average concentration. This difference in terms of leaching potential could be caused by the organic carbon content which was relatively low irrespective of the horizons for Rathangan compared to Clonroche. Soil organic carbon acts as an absorbent of a pesticide, therefore reducing the potential to freely leach to the groundwater (Wauchope et al., 2002). In addition, another difference noticed was that the Rathangan soil texture was not homogenous and had a high clay content which increased with depth for all horizons. According to Flury (1994) and Brown et al. (1999), chemical transport occurs as a preferential flow in soil with heterogeneous texture, like the one of Rathangan. This is consistent with the work of Kramers et al. (2012) who noticed that preferential flow is more likely to occur at this site. However, the simulation of preferential flow in PELMO is recent and there are limited studies to verify the ability of the model to simulate this type of chemical transport. Jarvis et al. (2003) conducted preliminary tests of the preferential process in PELMO for two clay soils. The authors showed that the results of macropore flow in PELMO were promising as they were in line with the one of MACRO but required further investigations. The pesticide leaching potential of the Elton scenario is higher than the one of Oak Park scenario. Elton compared to the Oak Park soil, is deep with low organic carbon and high clay content in the lower horizons. An analysis of the inputs to the Rathangan scenario (i.e., most vulnerable site) are presented in detail in **Fig. 6.** This highlights the importance of both pesticide and site inputs on model predictions.

The long term annual rainfall and average annual average temperature of the EU focus scenarios Okehampton and Hamburg fluctuated between 601 and 1401 mm and 5 and 12°C, respectively which were comparable to the Irish climatic conditions **(Fig. 5a**, **5b)**. However, effective rainfall (i.e., rainfall minus ET) is much lower for the Hamburg scenario compared to all the Irish sites **(Fig. 5c)**, while the effective rainfall for the Okehampton scenario is applicable to just some sites (Elton and Oak Park). This highlights the need for caution in applying these scenarios across different geographical locations. But the leaching pattern of the Okehampton and Hamburg scenarios compared to Irish site specific scenarios noticed in this study, should be viewed as the resulting outcome of a number of interaction processes, combining pesticide properties and management, soil and weather conditions (CARTER, 2000).

Three pesticides, MCPA, Mecoprop-P and Chlorothalonil were simulated based on the availability of pesticide site specific data and the results showed that all scenarios (EU FOCUS and Irish scenarios) had no leaching of Chlorothalonil **(Table 5)**. Chlorothalonil showed a high sorption potential in the four Irish sites with the soil sorption coefficient ranging from 978 to 2363 L/kg and these results were in the range of the average values (of 300-7000 L/kg) published in the FOOTPRINT database (FOOTPRINT, 2006); this indicated that this chemical is not available in the soil solution as it is strongly sorbed by the soil particles. In contrast to Chlorothalonil, the results of MCPA and Mecoprop-P indicated that these pesticides can leach with the possibility of exceeding the drinking water standard under the management practice described. The scenarios modelled in this study assumed a maximum application rate (and hence may be pessimistic, anecdotal evidence suggests most farmers may even only apply 70% of the recommended rate as a cost saving measure) based on the current maximum guideline of the Pesticide Control Service for the proposed use of MCPA and Mecoprop-P, consisting of two application doses to grassland (2 × 1.65 kg/ha in grassland and 2 × 1.4 kg/ha) and the maximum individual dose to spring cereals (2.1 kg/ha and 1.98 kg/ha). The simulated results highlight the need for customized applications based on individual pesticide properties and site conditions. In this study, MCPA leached more than Mecoprop-P in 4 out of 6 scenarios, based on the highest concentration. This finding is interesting as the sorption values of Mecoprop-P is lower than the one of MCPA and differed by 12.76 and 27.33 % for grassland and tillage, respectively **(Table 2)**. The difference between Mecoprop-P and MCPA is likely to be due to the fact that the degradation rate of Mecoprop-P is higher and may reduce its leaching potential compared to MCPA. The findings of this study were based on site specific sorption data while the degradation values where obtained from literature and therefore, field degradation studies in Irish conditions may help to reduce the uncertainties of the model predictions (Klein, 2000; Dubus, 2003).

4.3 Implications

According to the Council Directive 91/414/EEC, the determination of the predicted environmental concentration is a key step of the risk assessment for groundwater contamination by pesticides (CEC, 1994). In this study, the parameterisation and simulation of the EU Okehampton and Hamburg scenarios and Irish site specific scenarios showed that more chemical was predicted to leach with the former scenarios **(Table 5)**. This highlights the conservative nature of the EU FOCUS scenarios compared to Irish site specific scenarios and from an environmental point of view, will assist in reducing the risk of groundwater contamination.

5. Conclusion

A number of site specific scenarios were parameterised and validated with percolation and soil tension in this paper. The aim of this study was to compare simulate leachate levels at site specific scenarios to the EU FOCUS scenarios applied to the same sites. The parameterisation and simulation of the EU Okehampton and Hamburg scenarios and Irish site specific scenarios showed that the former overestimated the leaching potential. From this modelling exercise, it can be concluded that the FOCUS scenarios are more conservative than the site-specific scenarios, and therefore providing a risk buffer in terms of certification of products and hence might be regarded as positive from an environmental point of view. This indicates that the use of EU FOCUS scenarios under Irish specific conditions ensures the protection of Irish groundwater from pesticides. Among the four sites evaluated, Clonroche was identified as the least vulnerable area while Rathangan had the highest vulnerability to pesticide loss. Additional data on pesticide transport and site specific field studies (in particular, pesticide soil degradation studies) will provide greater insight into the risk of groundwater contamination by pesticides in Ireland.

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Fig. 1. Schematic diagram of the method used to assess the risk of pesticide leaching.

Fig. 2. Percolate validation based on the lysimeter experiments for (a) Oak Park, (b) Clonroche, (c) Rathangan and (d) Elton.

Fig. 3. Soil tension validation for Oak Park.

[Soil tension data source: Premrov et al., 2010; Used with permission.]

Fig. 4. Organic carbon, clay silt and sand content in A, B and C horizons

Fig. 5. Analysis of climate data (yearly minimum and maximum values shown in bars). (a) precipitation, (b) annual average temperature and (c) effective rainfall.

Fig. 6. Sensitivity analysis (± 10% from baseline model) of the model inputs for Rathangan scenario (i.e., most vulnerable scenario).

List of tables

Table 1

Physical properties of the soils selected (continued next page)

Scenarios	Thickness [a]	Texture [b]	Clay [b] (%)	Silt [b] (%)	Sand [b] (%)	pH [b]	Bulk dens [c] (kg/L)	Org C [d] (%)	Structure [e]	Drainage [f]
Oak Park	20	Sandy loam	11	23	67	6.6	1.49	2.9	Single grain	Very good
	25	Sandy loam	12	20	68	7.8	1.49	1.9	Fine granular	
Clonroche	20	Loam	17	39	44	6.5	1.29	4.9	Fine granular	Good
	25	Loam	25	37	38	7.3	1.62	2.38	Coarse granular	
	45	Loam	14	41	45	7.1	1.4	1.76	Fine angular blocky	

Table 1 (Continued)

Scenarios	**Thickness** [a]	**Texture** [b]	**Clay** [b] **(%)**	**Silt** [b] **(%)**	**Sand** [b] **(%)**	**pH** [b]	**Bulk dens** [c] **(kg/L)**	**Org C** [d] **(%)**	**Structure** [e]	**Drainage** [f]
Rathangan	20	Loam	19	37	44	6	1.13	3.37	Fine subangular blocky	Poor
	30	Sandy clay loam	24	28	48	6.3	1.57	1.66	Moderate subangular blocky	
	20	Clay loam	28	30	42	6.5	1.66	0.68	Coarse subangular blocky	
	30	Clay loam	29	39	32	6.7	1.83	0.67	Very Coarse subangular blocky	

Table 1 (Continued)

Scenarios	Thickness [a]	Texture [b]	Clay [b] (%)	Silt [b] (%)	Sand [b] (%)	pH [b]	Bulk dens [c] (kg/L)	Org C [d] (%)	Structure [e]	Drainage [f]
Elton	20	Loam	17	35	48	6.2	1.08	3.98	Fine subangular blocky	Good
	30	Silt loam	14	50	38	6.8	1.52	1.98	Moderate subangular blocky	
	40	loam	23	30	47	6.9	1.49	1.13	Coarse angular blocky	

Sources: [a] Adjusted (to fit the model file) based on Kramers et al., 2012 and Brennan et al., 2010. [b] From Kramers et al., 2012 and Brennan et al., 2010. [c] PEDOSPHERE, 2011. [d] organic matter divide by 1.72 as suggested by Schulte and Hopkins 1996 . [e] Kramers et al., 2012; [f] Brennan et al., 2010.

Table 2

Pesticide sorption, degradation and volatilisation properties used during the simulations

Pesticides (IUPAC names)	**Koc in L/kg (Freundlich exponent: 1/n) [a]**								**DT_{50} in days [b]**	**Henry's constant in Pam3/mol [b]**	**Vapour pressure in Pa [b]**	**Soil photolysis rate in 1/day**
	Oak Park		*Clonroche*		*Rathangan*		*Elton*					
	Grass	Tillage	Grass	Tillage	Grass	Tillage	Grass	Tillage				
MCPA (4-chloro-o-tolyoxyacetic Acid)	50 (0.91)	42 (0.91)	108 (0.90)	-	49 (0.95)	-	52 (0.97)	-	24	5.50×10^{-5} (at 25 °C)	0.0004 (at 25 °C)	[c] 0.027
Mecoprop-P [(R)-2-(4-chloro-o-tolyloxy)-propionic acid]	44 (0.96)	30 (0.98)	-	-	-	-	-	-	8	5.70×10^{-05} (at 25 °C)	0.00023 (at 25 °C)	[d] 0.02
Chlorothalonil (tetrachloroisophthalonitrile)	978 (0.74)	-	1279 (0.83)	-	1722 (0.88)	-	2363 (0.84)	2149 (0.93)	22	2.50×10^{-02} (at 25 °C)	0.076 (at 25 °C)	[e] Not considered (unlikely to occur)

Sources: [a] Piwowarczyk, 2013; [b] FOOTPRINT database, 2006. [c] European commission 2008, [d] European commission 2003 [e] European commission 2006 (-) Not available.

Table 3

Pesticide application dose.

Pesticides	**Multiple application (kg/ha)**	**Max application (kg/ha)**	**Average application (kg/ha)**	**Crop**
[a]MCPA	1.65 (× 2)	2.1	1.289	Grass, spring cereals
[a]Mecoprop-P	1.4 (× 2)	1.98	0.840	Grass, spring cereals
[b]Chorothalonil	-	-	1.2	-

Sources: [a] Personal communication, Irish Pesticide Control Service (2012); [b] Pesticide Survey (DAFF, 2003; DAFF, 2004); (-) not available.

Table 4

Model efficiency (EF) for the selected parameters.

Phases	Description	Value used	EF
Parameterization	Initial water content in %	30	-1.96
	Mid season	1	
	Late season	1	
	Root depth in cm	45	
	Evapotranspiration depth in cm	15	
	Dispersion length in cm	5	
	Thickness of layers in cm	2.5	
Sensitivity analysis	Initial water content +10 %	0.33	-1.96
	Initial water content -10 %	0.27	-1.96
	Mid season + 10 %	1.1	-1.96
	Mid season - 10 %	0.9	-1.96
	Late season + 10 %	1.1	-1.96
	Late season - 10 %	0.9	-1.96
	Root depth +10 %	49.5	0.96
	Root depth -10 %	40.5	0.96
	Evapotranspiration depth + 10%	16.5	-1.96
	Evapotranspiration depth - 10%	13.5	-1.96
	Dispersion length + 10%	5.5	-1.96
	Dispersion length - 10%	4.5	-1.96
	Thickness of layers (modification from 2.5 to 5 cm)	5	-0.39
	Inclusion of Macropore		-2.01

Table 5

Comparison of FOCUS scenarios to Irish site specific scenarios (Continued next page)

Scenarios	Crop	Pesticide	Highest concentration (HC) in µg/L	Average concentration (AC) in µg/L	Solute outflow (SO) in kg/ha	[1]Year breach the DWS	% Above site specific HC	% Above site specific AC	% Above site specific SO
Oak Park	Grass	MCPA	6.34E-01	3.15E-02	1.85E-02	4			
	Tillage	MCPA	1.16E-01	1.06E-03	5.84E-04	17			
Okehampton	Grass	MCPA	1.91E+01	5.11E+00	9.45E-01	2	96.7	99.4	98
	Tillage	MCPA	1.83E+00	2.64E-01	5.00E-02	3	93.7	99.6	98.8
Hamburg	Grass	MCPA	2.28E+01	8.79E-01	5.00E-01	2	97.2	96.4	96.3
	Tillage	MCPA	2.04E+00	4.11E-02	2.30E-02	4	94.3	97.4	97.5
Clonroche	Grass	MCPA	2.33E-02	6.76E-04	6.08E-04	none			
Okehampton	Grass	MCPA	8.32E-01	1.67E-01	3.12E-02	3	97.2	99.6	98.1

Table 5 (Continued)

Scenarios	**Crop**	**Pesticide**	**Highest concentration (HC) in µg/L**	**Average concentration (AC) in µg/L**	**Solute outflow (SO) in kg/ha**	**[1]Year breach the DWS**	**% Above site specific**		
							HC	**AC**	**SO**
Hamburg	Grass	MCPA	9.66E-01	2.09E-02	1.25E-02	4	97.6	96.8	95.2
Rathangan	Grass	MCPA	1.18E+01	5.60E-01	4.26E-01	2			
Okehampton	Grass	MCPA	2.48E+01	7.23E+00	1.35E+00	1	52.4	92.3	68.5
Hamburg	Grass	MCPA	2.94E+01	1.32E+00	7.38E-01	1	59.9	57.5	42.2
Elton	Grass	MCPA	4.94E+00	2.98E-01	1.74E-01	1			
Okehampton	Grass	MCPA	2.41E+01	7.21E+00	1.35E+00	1	79.5	95.9	87.1
Hamburg	Grass	MCPA	2.86E+01	1.31E+00	7.34E-01	1	82.7	77.3	76.3

Table 5 (Continued)

Scenarios	Crop	Pesticide	Highest concentration (HC) in µg/L	Average concentration (AC) in µg/L	Solute outflow (SO) in kg/ha	[1]Year breach the DWS	% Above site specific		
							HC	AC	SO
Oak Park	Grass	Mecoprop-P	8.20E-02	7.29E-04	4.52E-04	none			
	Tillage	Mecoprop-P	3.83E-01	3.70E-03	2.10E-03	10			
Okehampton	Grass	Mecoprop-P	5.99E-01	4.29E-02	1.29E-02	3	86.3	98.3	96.5
	Tillage	Mecoprop-P	1.33E+00	6.68E-02	1.93E-02	3	71.2	94.5	89.1
Hamburg	Grass	Mecoprop-P	6.29E-01	1.45E-02	8.65E-03	5	87.0	95.0	94.8
	Tillage	Mecoprop-P	2.46E+00	1.32E-02	8.28E-03	5	84.4	71.9	74.7
[2]All scenarios	Grass	Chlorothalonil	0	0	0	none	0	0	0

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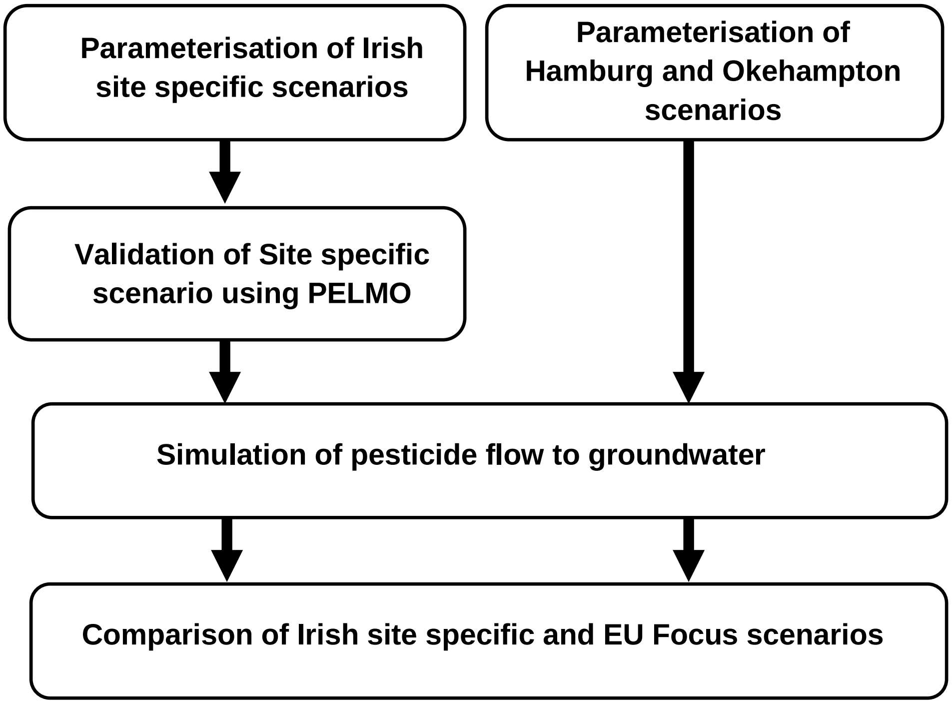
[1] Number of years (over a 26 years period) where pesticide concentration is predict the first time to breach the drinking water standard DWS (i.e., simulated pesticide concentration is equal or beyond 0.1 µg/L). [2] Oak Park, Clonroche, Rathangan, Elton, Hamburg and Okehampton scenarios exhibited no leaching potential with Chlorothalonil.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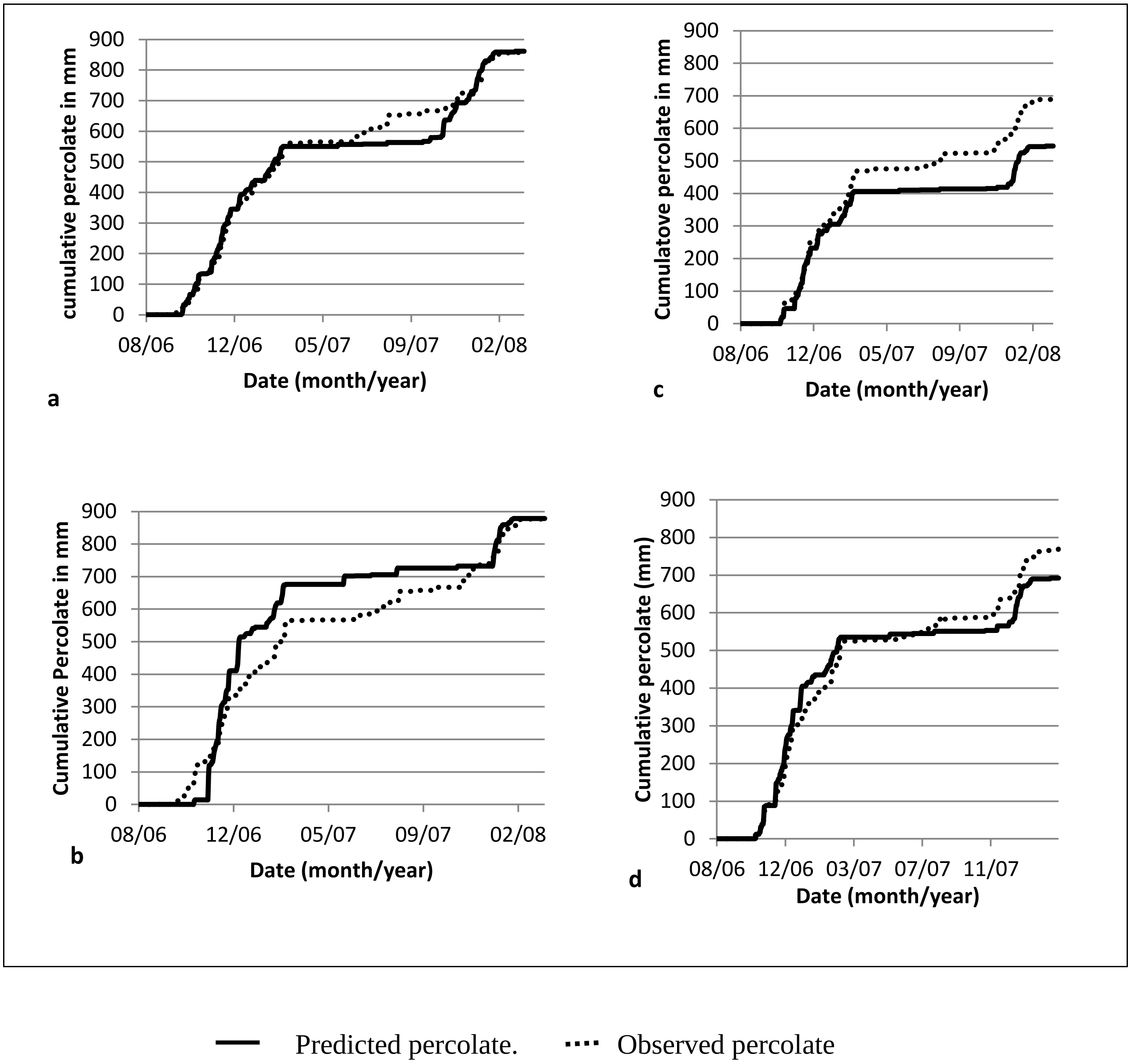
Parameterisation of Hamburg and Okehampton scenarios
Validation of Site specific scenario using PELMO
Simulation of pesticide flow to groundwater
Comparison of Irish site specific and EU Focus scenarios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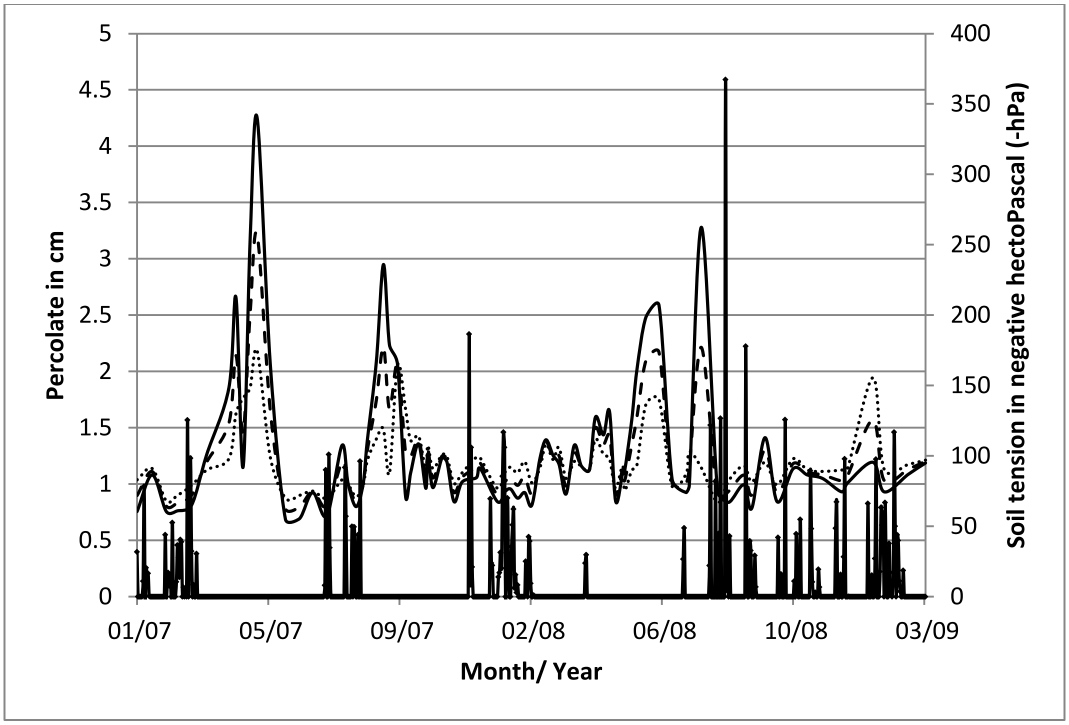

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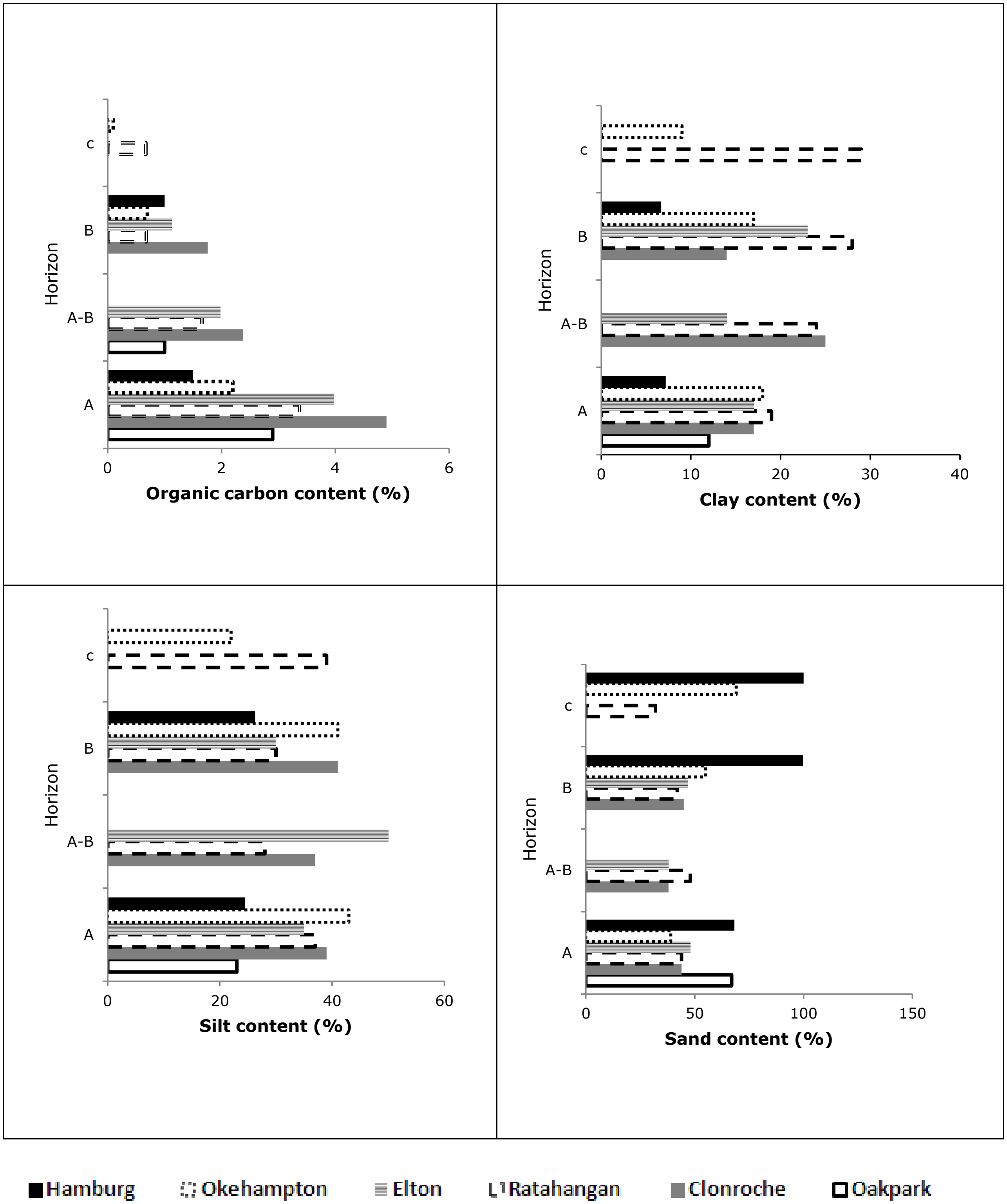
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Clay content (%)
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Silt content (%)
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B
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Sand content (%)
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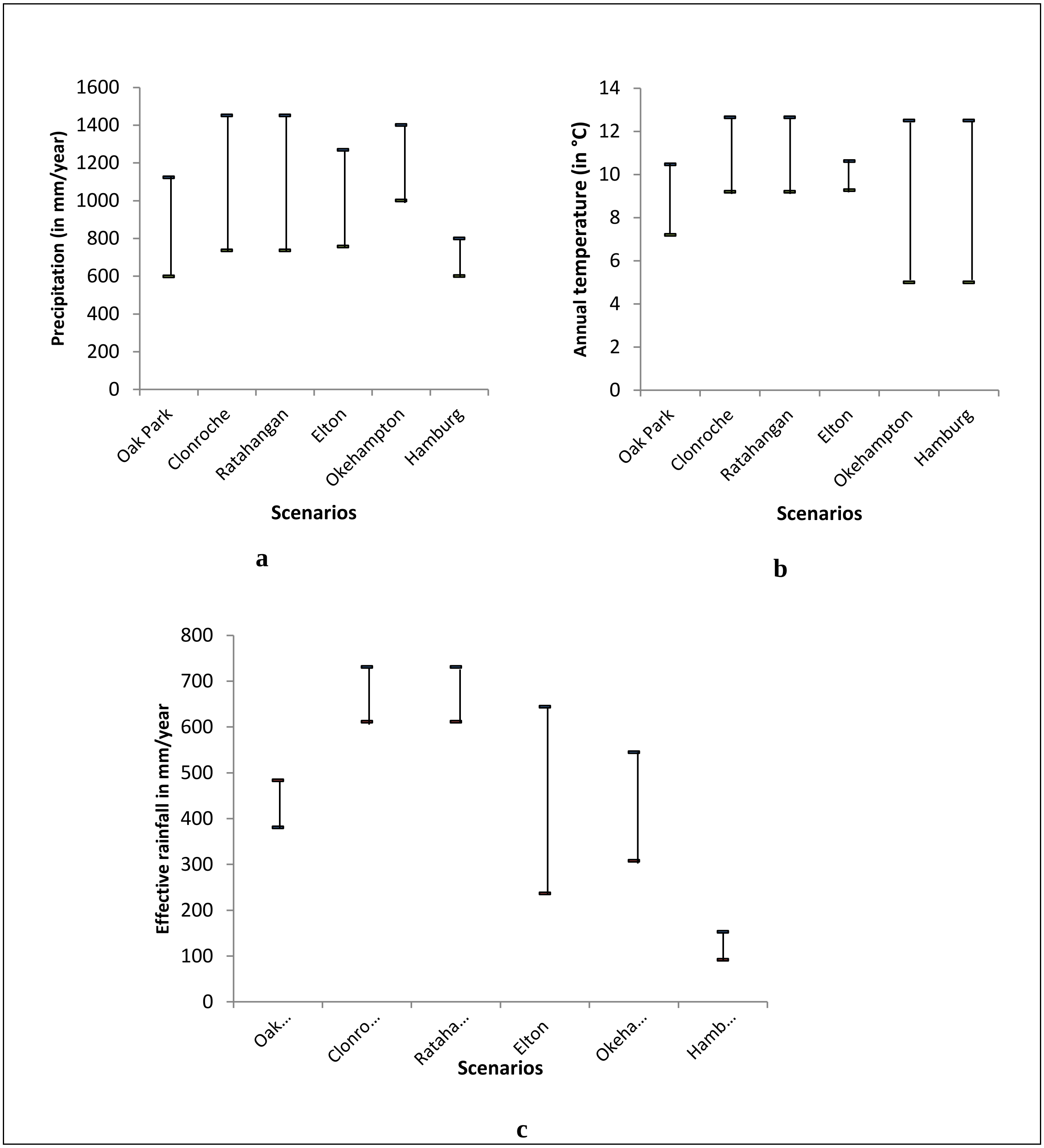
⬚ Okehampton
▤ Elton
Ratahangan
■ Clonroche
□ Oakpark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1400
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600
400
200
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Oak Park
Clonroche
Ratahangan
Elton
Okehampton
Hamburg
Scenarios
a
Annual temperature (in °C)
14
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6
4
2
0
Oak Park
Clonroche
Ratahangan
Elton
Okehampton
Hamburg
Scenarios
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Effective rainfall in mm/year
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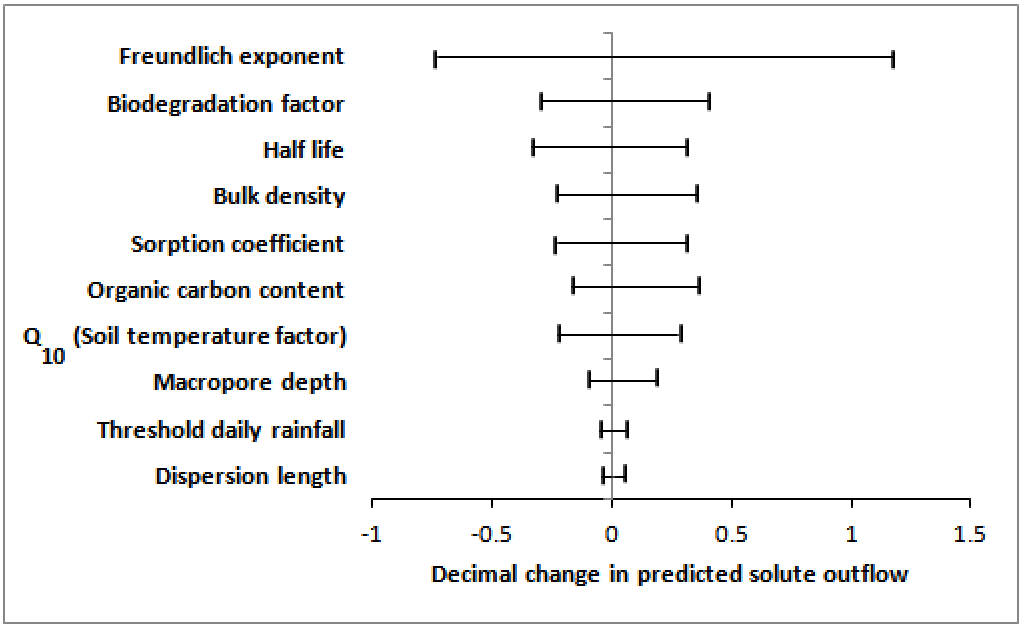
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Biodegradation factor
Half life
Bulk density
Sorption coefficient
Organic carbon content
Q_{10} (Soil temperature factor)
Macropore depth
Threshold daily rainfall
Dispersion length
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-0.5
0
0.5
1
1.5
Decimal change in predicted solute outflow