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HardSPEC

A First-tier Model for Estimating Surface- and Ground-Water Exposure resulting from Herbicides applied to Hard Surfaces

Model Overview and Technical Guidance for Users of HardSPEC

by

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With a section by staff of the **Chemicals Regulation Division** on regulatory use.

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Foreword

This document is a short version of the full Guidance Document Report (Hollis *et al*, 2017) issued by the Chemicals Regulation Division (CRD) which provides a description and explanation of HardSPEC, an aquatic exposure model for pesticides used on hard surfaces. It is intended for model users who do not want to investigate the full detail of scenario and model development but still require an overview of the various scenarios covered and guidance on how to use the model.

Development of the HardSPEC model was funded primarily by the former Pesticides Safety Directorate (PSD), through the Department for Environment, Food and Rural Affairs (DEFRA, formerly MAFF). Its development also made extensive use of field and laboratory studies which were sponsored by several organisations: Department of the Environment, Transport and the Regions; The Environment Agency of England and Wales; UK Water Industry Research Association Ltd; Agrichem International Ltd; Bayer CropScience through its predecessor companies AgrEvo UK Ltd and Rhône-Poulenc Agriculture Ltd.; Dow AgroSciences; The Scotts Company (UK) Ltd; Monsanto Agricultural Company; Novartis Crop Protection. The authors would like to thank representatives of all the sponsoring organisations for their invaluable help and advice throughout the projects reported or referred to here.

Opinions expressed within the report are those of the authors and do not necessarily reflect the opinions of the sponsoring organisation. No comment within this report should be taken as an endorsement or criticism of any herbicide compound or product.

Reference to this report should be made as follows:

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1 BACKGROUND TO THE MODEL DEVELOPMENT

Herbicides are commonly used for weed control on non-agricultural surfaces such as footpaths, road edges and railway track beds. In contrast to the fate of pesticides applied in the soil-based agricultural environment, there is little information on the dissipation and re-distribution of herbicides used in 'hard surface' environments and any associated contamination of receiving waters. Prior to 2004, in the absence of such information, the UK Pesticides Safety Directorate (now known as the Health and Safety Executives Chemicals Regulation Division) used a crude exposure assessment that assumed all of the herbicide applied on hard surfaces 'not intended to bear vegetation' is lost to surface waters in a volume equivalent to 25mm of rainfall.

To redress the paucity of information about the transfer of herbicides from hard surfaces to water, a series of projects were carried out between 1997 and 2004 to investigate and model the losses of herbicides from a variety of relevant man-made surfaces. The objectives of these studies were:

- To generate quantitative information on the amounts and concentrations of herbicides impacting on water resources when applied in specific realistic situations.
- To develop an initial understanding of the dissipation mechanisms operating in such environments.
- Based on the knowledge derived from these studies, to develop a model that could be used to undertake a first-tier estimate of surface- and ground-water exposure to assist the risk assessment process for herbicides applied to hard surfaces.

An initial version of the 'first-tier' model was completed in June 2000 (Hollis *et al*, 2000) and was based on study results available prior to that date. This initial version considered two surface water scenarios, one for an urban runoff situation and one for a rural major road. Both scenarios incorporated a sub-routine for calculating wash-off from individual hard surfaces and a surface water fate sub-routine for dissipation in the surface water body associated with each scenario. There were three main problems with this initial version of the first-tier model:

- Although the model enabled users to estimate exposure in surface waters, no routines for estimating ground-water exposure were included. Local contamination of ground-water by herbicides used along railway tracks has been highlighted as being a particular concern of the Environment Agency.
- The sub-routines for predicting wash-off from individual hard surfaces were modelled using empirically-derived factors based on a set of controlled wash-off studies (Shepherd &

Heather, 1999) using a set of six herbicide compounds. Such an approach meant that there was great uncertainty when extrapolating model results to other herbicide compounds.

- The sub-routines for predicting fate in surface water bodies produced estimates of daily concentrations in the aqueous phase only and for a period of only 5 days after application. This meant that any environmental risk-assessment based on such exposure calculations could only be carried out in relation to acute toxicity values and then only based on aqueous exposure.

In order to address these limitations, further development of the model was carried out, along with additional studies to characterise the potential for contamination of ground-water following herbicide application to a railway (Ramwell *et al*, 2001), the inherent sorption potential of different types of hard surface (Ramwell, 2002) and the organic carbon content of railway ballast. In 2004 the revised model was accepted for regulatory use as a first tier assessment of aquatic exposure resulting from use of herbicides on Hard Surfaces. To support this use, a document was published describing the model together with a summary of the results of all previous studies carried out to support its development (Hollis *et al*. 2004). Subsequent use of the model has identified a number of minor 'bugs', as well as the need to modify and expand the existing scenarios. A new version of the model was subsequently released. A revised Guidance Document (Hollis *et al*, 2017) that updates the 2004 report including description of the additional scenarios (railway surface water and domestic use), modification of the urban pond scenario, an initial evaluation of the accuracy of model predictions and an outline of how to use the revised model software has also been released.

This document is a short version of the full Guidance Document. It is intended for model users who do not want to investigate the full detail of scenario and model development but still require an overview of the various scenarios covered and guidance on how to use the model.

2 MODEL OVERVIEW

Herbicides are applied to hard surfaces in urban, suburban and rural locations but the amounts of herbicide applied and methods of application will differ depending on the application scenario and the surface types involved. In addition, exposure estimates are required for both surface- and ground- water resources and the scenarios of concern for these two situations are very different. To allow for these differences, six exposure scenarios have been defined:

1. **Suburban (domestic use) Stream.** A surface water stream receiving surface drainage from a suburban catchment within which herbicides are applied to some hard surface areas on domestic properties.
2. **Urban Stream.** A surface water stream receiving surface drainage from an urban catchment within which the hard surface areas drain via gully pots.
3. **Urban Pond.** A pond receiving surface drainage waters from an urban catchment within which the hard surface areas drain via gully pots. This scenario is intended to represent the use of collecting ponds within Sustainable Urban Drainage Systems (SUDS).
4. **Major Road Stream.** A surface water stream receiving surface drainage from a major road in a rural setting where the hard surface areas drain via gully pots. The stream also receives drainage from an adjacent 1ha agricultural field.
5. **Railway Groundwater.** The abstraction point of a local groundwater body that receives herbicide leached from a double railway track which crosses the groundwater catchment.
6. **Railway Ditch.** A ditch adjacent to a railway embankment receiving water which has leached through railway ballast as well as spray drift from special “spray trains” running up and down the track.

2.1 Generic realistic worst case characteristics of all scenarios

In developing these six scenarios, a set of basic assumptions for herbicide application and weather patterns were established to characterise a generic realistic worst-case situation:

- Herbicides are applied in the early spring (March or April), except in the domestic use scenario when they are assumed to be applied in May.
- Herbicides are applied in a continuous swath, rather than spot-applied.
- A significant rainfall event occurs 24 hours after herbicide application.
- Rainfall amounts are representative of a ‘wet quartile’ year.
- There is no retention or dissipation of herbicide within gully pots.

2.2 Scenario-specific realistic worst-case characteristics

All other scenario characteristics are scenario-specific although they are based on real-world situations. They are fully described in Hollis *et al*, 2017 but an overview of the realistic worst-case conditions associated with them is given below:

2.2.1 Catchment Characteristics

- 67.5 % of the **urban catchment** comprises hard surfaces (based on data from Milton Keynes).
- The **suburban (domestic use) catchment** represents a 10 ha suburban development where almost all the properties are owner-occupied, detached or semi-detached houses (identified by surveys as a worst-case for likely herbicide usage). 99% of houses along the road network have frontages to it and those frontages all have a hard surface coverage based on an estimated average of the available data from published surveys.
- In the **groundwater catchment**, railway ballast directly overlies aquifer bedrock with shallow groundwater. This represents a 99.8th percentile worst-case for aquifer vulnerability.
- In the **railway surface water catchment** there is a ditch directly adjacent to the embankment on which the railway runs.

2.2.2 Herbicide application

Table 1 gives a summary of the worst-case application methods for each scenario. In addition:

- With the exception of the suburban (domestic use) scenario, all herbicide is applied in a single day (even in the urban scenario).
- In the **suburban scenario** 10% of all households apply herbicides to front gardens during an 18 day rain-free period that represents a 1 in 10 year event (a 90th percentile longest period for application). This pattern is supported by survey data.
- With the exception of the railway scenario, all herbicide is assumed to be applied either as a band-spray to pavement / roadside edges or in other relevant areas as a frequent spot-spray to a heavy weed infestation thus targeting most joints or cracks in individual hard surface types. Although this maximises the amount of compound applied, it means that vegetation intercepts 10% before it reaches any hard surface.
- In the **railway scenario**, there is a maximum spray target area because both ‘up’ and ‘down’ sets of tracks are sprayed and, as a first tier assessment it is assumed that herbicide is applied to 100% of the target area.

Table 1. Summary of worst-case application assumptions for each HardSPEC scenario, excluding Domestic Usage.

Scenario	Total road & pavement area draining to gully pots (m^2)	Application type	Surface area receiving spray (m^2)	As % of total application load	% of total road & pavement area sprayed	Assumptions
Urban	22400	Strip spray	1220.8	89.0	5.45	Applied as a continuous 0.3 m wide swath along the kerbs on either side of roads
		Spot spray	151.2	11.0	0.675	Applied to 2% of pavement area not affected by the strip spray
Rural Road	716	Strip spray	78.0	100.0	10.89	Applied as a continuous 0.3 m wide swath along the kerbs on either side of the road
Railway	**Total Ballast & track area (m^2)**				**% of total track area sprayed**	
	774.7	Radiarc nozzles	774.7	100.0	100.00	Applied using both downwards & sideways nozzles to both 'Up' & 'Down' tracks

2.2.3 Spray drift

- With the exception of the suburban (domestic use) scenario (where there are no spray drift inputs to surface water) and the railway scenario, all spray drift inputs are based on the 90th percentile values from BBA, 2000. This assumes: All plants up to the edge of the water body are <50 cm tall; There is only 1 m from the edge of the spray application to the start of the water body.
- In the **railway scenario**, drift from the spray train is based on the worst-case wind direction (the same direction as that of the sideways pointing nozzles nearest to the ditch) and the amount is based on experimental data for an absolute worst-case wind speed of 12 miles hr^{-1} (5.36 m s^{-1}).

2.2.4 Rainfall

- The spring rainfall pattern is a real one and includes the following characteristics based on long term weather data for a UK area of average wetness:
- A 75th percentile wettest daily rainfall event occurs on the day after application.
- There is a total of 16 mm of rainfall over the 6 days following application which represents a 75th percentile shortest period for such an amount.
- The total rainfall during the 3 months after application represents a 75th percentile largest amount.

2.2.5 Catchment hydrology

- Percentage rainfall:runoff coefficients for different surface types in the urban, suburban and major road catchments are based on measured data related to the application months of March, April and May and include evapotranspiration losses relevant to those months, thus giving the lowest realistic runoff volumes for dilution of washed off herbicide loads.
- All herbicide loads washed off individual surfaces in the urban, suburban and major road catchments move to the catchment stream on the day of wash-off (there is no retention within the catchment), except in the suburban (domestic use) catchment where a small percentage is lost from ‘leakage’ through the cracks or joints in concrete or brick paving surfaces.
- In the **suburban catchment**, 95% of houses along the road network have frontages that drain directly to it and then via storm drains or culverts to a local stream (a realistic worst case for wash-off to semi-natural surface water bodies).

- In the **railway surface water catchment** runoff alternative, 88% of the total load leaching out of the railway formation contributes to runoff down the embankment side nearest to the ditch and, as a first tier assessment it is assumed that there is no attenuation of herbicide loads during runoff to the surface water body.

- In the **railway surface water catchment** leaching alternative, there is no attenuation of loads leached out the railway formation during transport in the unsaturated zone and there is no lateral advection-dispersion during transport in the saturated zone.

- In the **groundwater scenario**, herbicide concentrations at the wellhead are calculated with a one dimensional advection-dispersion model: there is no lateral advection-dispersion (i.e. perpendicular to the hydraulic gradient).

2.2.6 Surface Water Dynamics

- The **streams and ditch** are small 1 m wide surface water bodies with characteristics similar to those of the FOCUS_{sw} bodies although in the urban and suburban scenarios they have a length of 316 m, consistent with a 10 ha catchment area. These characteristics minimize the initial volume of water that is available for dilution of incoming herbicide loads.

- The dimensions of the **urban pond** are based on the design specifications recommended by the Construction Industry Research and Information Association (CIRIA) using a realistic combination of soil type and climate designed to give the realistic smallest initial water volumes at the start of the spring period and maximum permissible outflow from the pond. This ensures a realistic minimum water volume for dilution of incoming herbicide wash-off loads.

- Only 2/3 of spray drift inputs to all relevant surface water bodies are available for partitioning. This is the same as in the ‘STEPS1-2 in FOCUS’ model and is based on experimental observations (Linders *et al.*, 2003).

- Concentrations in the water bodies resulting from spray drift on the day of application are calculated before any partitioning or advective losses occur at the end of the time step.

- In the **stream scenarios**:
  - Only 1/3 of herbicide wash-off inputs to the stream are available for partitioning.
  - The water residence time in the stream is 24 hrs as compared to a calculated maximum residence time of 8 hrs in all the FOCUS surface water stream scenarios (Linders, *et al*, 2003).

- In the **roadside scenario**, dilution of herbicide wash-off inputs comes only from the adjacent agricultural field. There is no dilution derived from ‘up-stream’ water inputs.
- In the **urban pond** scenario, each daily concentration in the water body is calculated before any partitioning or advective losses occur at the end of the time step.

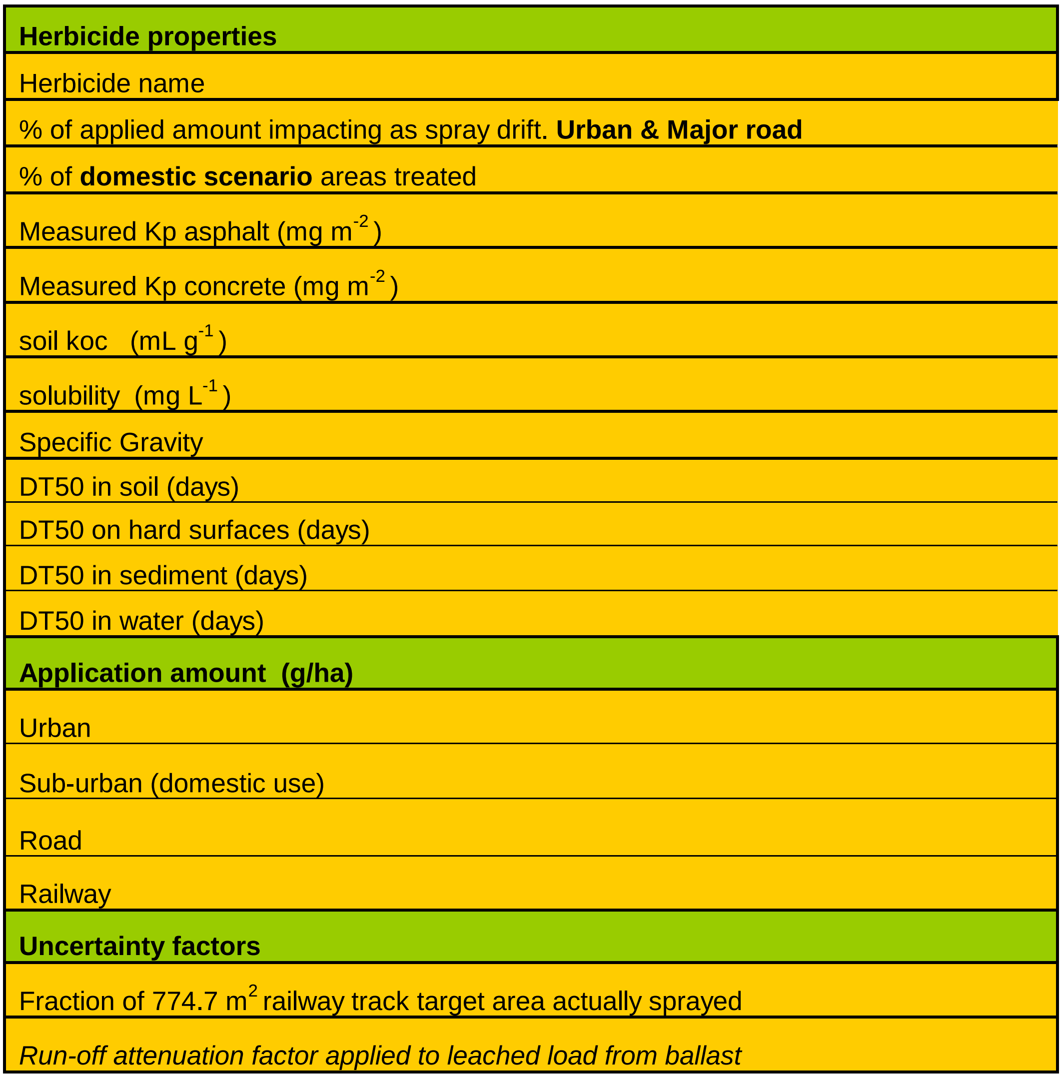
3 USE OF THE EXPOSURE MODELS

HardSPEC is implemented as an MS Excel work-book and has a modular structure comprising 11 worksheets each dealing with a different function of the model. The first two worksheets, “**Herb_props**” and “**OUTPUT**” are for users to input data to the model and view model results. The next 4 worksheets: “**Domestic_Use_scenario**”, “**Urban_scenario**”, “**Major_scenario**” and “**Railway_scenario**” define the fixed scenario surface characteristics whilst the following 5 worksheets: “**Losses_BR**”, “**Masses lost per 0.5mm rain**”, “**Groundwater model**”, “**Railway surface water**” and “**Losses_AR**” each calculate different aspects of herbicide fate. All worksheets except the Herb_props are protected, although cell contents can be viewed and copied into other workbooks or applications.

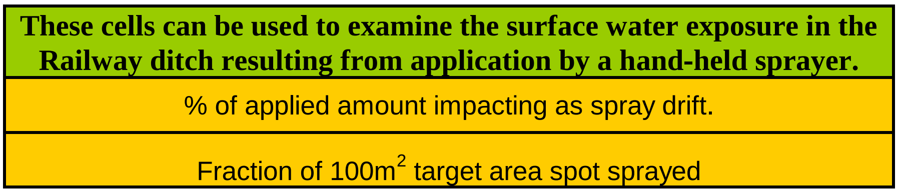
The following sections provide an overview of how to use the model and the contents of each of its component worksheets. Finally, there is a brief statement of the regulatory context within which the model is used.

3.1 Worksheet "Herb_props":

This sheet enables the user to input the substance properties that are required to drive the model (for historical reasons the model uses the term 'herbicide' rather than 'substance'; from here on the term 'substance' is used). These are the only direct user-inputs to the model and comprise the following:



Herbicide properties
Herbicide name
% of applied amount impacting as spray drift. **Urban & Major road**
% of **domestic scenario** areas treated
Measured Kp asphalt (mg m^{-2})
Measured Kp concrete (mg m^{-2})
soil koc (mL g^{-1})
solubility (mg L^{-1})
Specific Gravity
DT50 in soil (days)
DT50 on hard surfaces (days)
DT50 in sediment (days)
DT50 in water (days)
Application amount (g/ha)
Urban
Sub-urban (domestic use)
Road
Railway
Uncertainty factors
Fraction of 774.7 m^2 railway track target area actually sprayed
Run-off attenuation factor applied to leached load from ballast



These cells can be used to examine the surface water exposure in the Railway ditch resulting from application by a hand-held sprayer.
% of applied amount impacting as spray drift.
Fraction of $100m^2$ target area spot sprayed

Some of these input parameters, such as water solubility and specific gravity (relative density), should be readily available to users. However many others, particularly those specific to hard surfaces such as the measured substance partition coefficient (Kp) on asphalt or concrete are unlikely to be available for most substances. In such cases, the model will use a default value or a calculation (estimate based on Koc). Other input parameters such as DT_{50} values need careful evaluation to ensure that they are compatible with the assumptions used in the model. The following paragraphs provide some guidance on the selection or derivation of such input parameters:

Percentage of the applied amount impacting as spray drift: ***Urban & Major Road Scenario.*** The model uses a default value of 2.8%, taken from the FOCUS Surface Water Scenario drift calculator (Linders *et al*, 2003). This is the value derived for a hand held application to a crop < 50 cm high and at a distance of 1 m from the edge of the 'crop' to the start of the water body. **Users should not alter this value unless they wish to examine the potential effect of buffer strips or ‘no spray’ zones on predicted surface water concentrations, in which case the alternative values used should be fully justified**.

Users should also note that if they reduce the percentage of applied amount impacting as spray drift, the amount reduced is calculated and added to the mass of substance falling on each hard surface type. In other words, it is assumed that the total amount of applied substance that is not intercepted by plants or is not lost in drift impacts on a hard surface. **When examining the potential impact of buffer strips or no-spray zones therefore, users should only consider changes to PECsw on the day of application and should be aware that PECsw on the subsequent day (the first rainfall event) may increase slightly as a result of the assumed increased hard surface loading.**

Percentage of areas treated: ***Domestic Use Scenario***. The model uses a default value of 10% based on confidential Electronic Point of Sale (EPoS) monthly sales information related to the likelihood of a significant rain-free period occurring during the peak sales month. It is well supported by data from a study of domestic usage within a small suburban catchment in York and **the value should not be changed unless strong evidence can be presented to show it is unrealistic for the substance under consideration**.

Measured Kp asphalt.

Measured Kp concrete.

These input parameters should be derived using the following steps:

1. If you are dealing with a substance that either

   a). Is subject to rapid hydrolysis, OR,

   b). Has a pH-dependent soil Koc,

   then you must carry out **a controlled wash-off study. The protocol for such a study is currently being finalized. In the interim, users needing to carry out the study should contact Dr. C. T. Ramwell, The Food and Environment Research Agency, Sand Hutton, York. YO41 1LZ (Email: carmel.ramwell@fera.co.uk; Tel: +44 (0)1904 462485).**

   Results from the study should then be used to calibrate the wash-off model. Future releases of the HardSPEC model will contain a module to allow such calibration but in the period before this version is available, Applicants should contact John Hollis (Email: hollises@btinternet.com: Tel: +44 (0)1727 823810) for assistance on calibration issues.

   If you are dealing with a substance that has a **wide range of soil Koc values as a result of its complex sorption behaviour (for example because it has a zwitterionic structure with both positive and negative charges on different atoms within the molecule and/or it shows evidence for the formation of metal-phosphonate complexes with metals including iron (III) and copper; this is not an exhaustive list of examples)**, then you must carry out **a surface-specific sorption study using the procedure described by Ramwell (2011), unless, as a result of step 1 above, the model has already been calibrated using the results of a controlled wash-off study,** in which case **no further work is necessary.**

   The resulting measured $Kp_{asphalt}$ and $Kp_{concrete}$ values should be inserted in cells C8 & C9 of the “Herb_props” worksheet.

2. For all other substances, you should **type in “not known” in each of cells C8 and C9** of the “Herb_props” worksheet. The model will calculate the $Kp_{asphalt}$ and $Kp_{concrete}$ values using the relationships with soil Koc derived as a result of the sorption study (Ramwell, 2002). These relationships are shown in Figure 1, below.

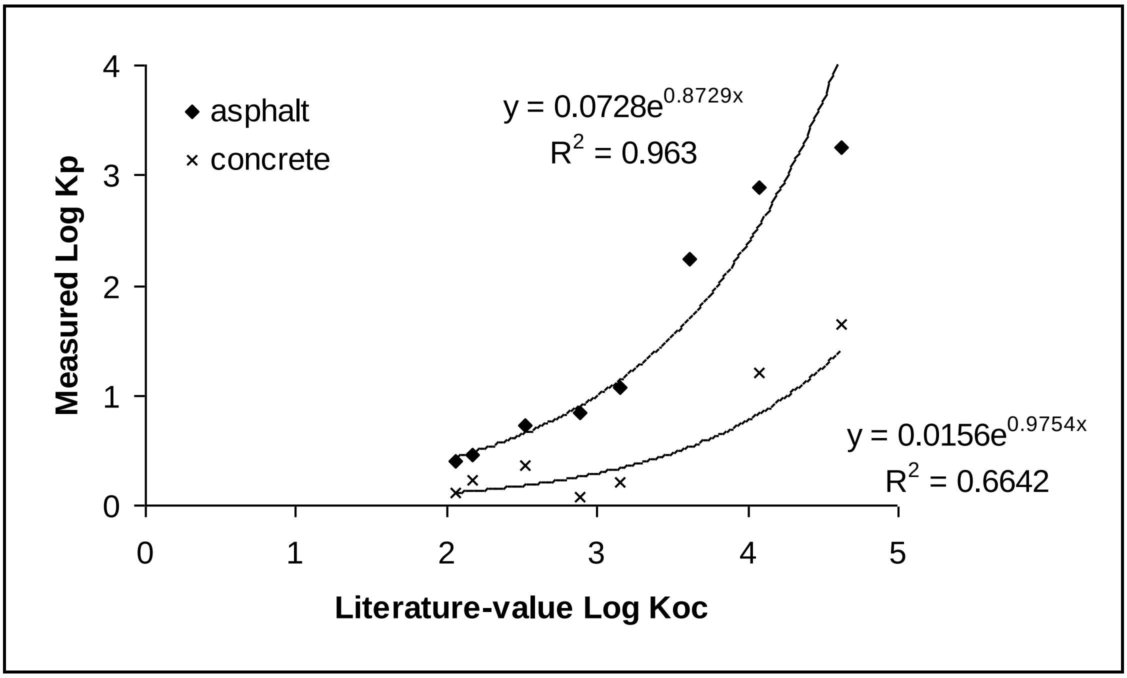


Figure 1 Relationship between measured Kp (mg m^{-2}) for concrete and asphalt and literature values of soil Koc (L kg^{-1}), (based on Ramwell, 2002).

In order to assess the possible errors resulting from using Koc-derived Kp values rather than measurements, the Koc relationship was used to estimate surface-specific Kp values for each of the six substances used in the controlled wash-off study (Shepherd & Heather, 1999) and, using the application rates and pesticide properties defined for that study, the wash-off sub-model was used to predict the masses lost in each 0.25 L of wash-off for each substance. The results were then compared to those produced using the measured Kp values for each substance. Statistical comparisons are given in Table 2 and overall comparisons (excluding results for glyphosate) are shown in Figures 2 and 3.

The statistical evaluation shows that, apart from glyphosate, there is virtually no difference in the accuracy of predictions for asphalt surfaces between those based on a measured $Kp_{asphalt}$ value and those based on a value predicted from the soil Koc. In contrast, for concrete surfaces, apart from atrazine, all substances show a slight decrease in accuracy of predictions when using a $Kp_{concrete}$ value estimated using soil Koc. However, as Figure 3 shows, the slight decrease in accuracy for concrete surfaces has no bias towards over- or under-estimation and, as the differences are so small, are unlikely to significantly change exposure results generated using the Kp estimation method.

Table 2 Statistical evaluation of the difference in accuracy of prediction of measured losses of the 5 test substance used in the controlled wash-off study (Shepherd & Heather, 1999), using measured Kp and Kp estimated from soil Koc

Substance	Model efficiency		Percentage error	
	Using measured Kp	Using estimated Kp	Using measured Kp	Using estimated Kp
	Asphalt			
atrazine	0.73	0.73	7.2	7.2
diuron	0.83	0.83	7.7	7.7
oryzalin	0.86	0.86	37.6	37.6
isoxaben	0.42	0.40	42.0	42.7
glyphosate	1.00	0.85	0.6	82.6
All substances except glyphosate	0.9885	0.9886	10.4	10.4
	Concrete			
atrazine	0.97	0.97	16.3	16.3
diuron	0.93	0.89	13.5	17.0
oryzalin	0.997	0.99	6.9	12.2
isoxaben	1.00	0.998	3.2	5.6
glyphosate	0.997	0.83	7.9	61.2
All substances except glyphosate	0.979	0.975	18.2	19.7

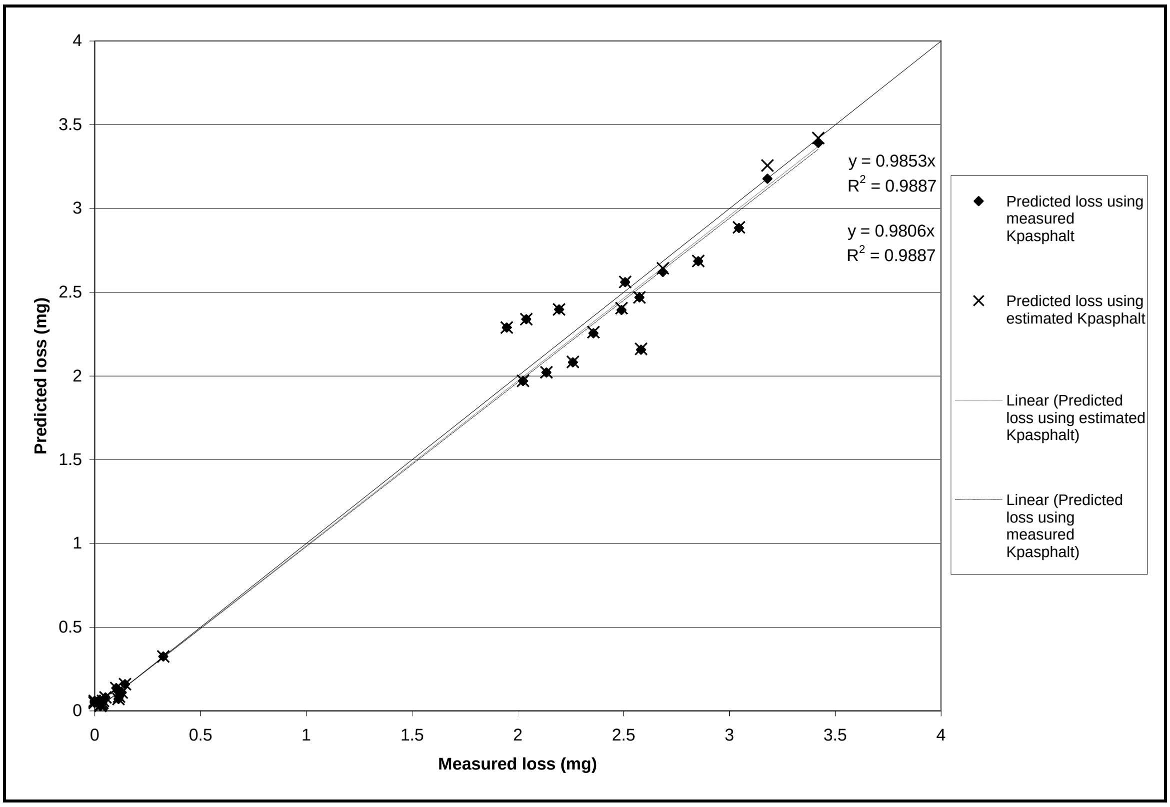


Figure 2. Comparison of measured and predicted losses (mg) from the controlled wash-off study on **asphalt** (Shepherd & Heather, 1999) using measured $Kp_{asphalt}$ and $Kp_{asphalt}$ predicted from Koc (glyphosate results excluded).

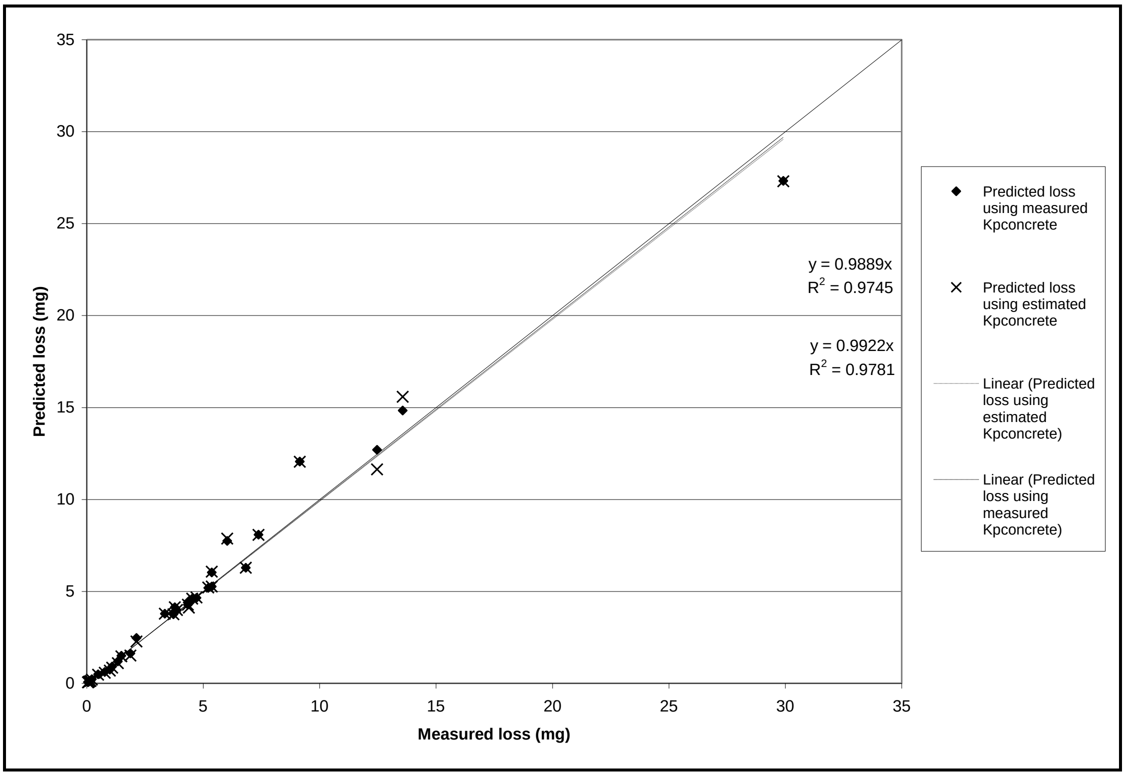


Figure 3. Comparison of measured and predicted losses (mg) from the controlled wash-off study on **concrete** (Shepherd & Heather, 1999) using measured $Kp_{concrete}$ and $Kp_{concrete}$ predicted from Koc (glyphosate results excluded).

Soil Koc.

Information on soil Koc of the substance for input to the model should be obtained from the standard regulatory dossier on soil sorption studies. When selecting an appropriate input value for soil Koc, users should refer, in the first instance, to the EFSA Conclusion or Review Report for the active substance for the value to be used in environmental exposure modelling. If necessary, for example in the situation that an EFSA Conclusion is unavailable or the Review Report gives insufficient detail of endpoints used in exposure modelling and the values used in the assessment for active substance approval are not known, users should refer to the latest “Generic Guidance for Tier 1 FOCUS Ground Water Assessments” Guidance Document for details on parameter selection.

Solubility.

Information on the solubility of the substance for input to the model should be part of the standard regulatory dossier. This should be available in the EFSA Conclusion or Review Report on the substance or from the physical/chemical properties section of the dossier.

Specific gravity.

The specific gravity of a substance is of particular relevance to the non-dissolved portion of the substance as simulated in the HardSPEC model. Wherever possible the specific gravity of the substance should be used. However, if the specific gravity of the substance is not known (noting that such information is not a standard data requirement in the EU and is unlikely to be available), the specific gravity of the formulation (typically expressed as relative density or tap density) should be entered into the model. This should be available from the physical/chemical properties section of the dossier. It should be noted that decreasing the specific gravity value is likely to result in higher PEC values.

DT_{50} in soil (days).

The model requires a value for the half life (i.e Single First Order DT_{50}) of the substance in soil. When selecting an appropriate input value for DT_{50} soil, users should refer in the first instance to the EFSA Conclusion or Review Report for the active substance for the value to be used in environmental exposure modelling. If necessary, for example in the situation that an EFSA Conclusion is unavailable or the Review Report gives insufficient detail of endpoints used in exposure modelling and the values used in the assessment for active substance approval are not known, users should refer to the latest “Generic Guidance for Tier 1 FOCUS Ground Water Assessments” Guidance Document for details on parameter selection.

DT_{50} on hard surfaces (days).

The model uses a single value for the half life of pesticides on all types of hard surface. If no surface-specific measured data for the substance is available, the user should type “**not known**” into **cell C14** and the model will use a value that is twice that of the soil half life value entered by the user. The various field and laboratory studies carried out to support model development suggested that degradation of applied substances does not occur on freshly made hard surfaces, but that, once exposed and weathered in ‘real world’ environments, hard surfaces are likely to acquire some potential for microbial degradation. Based on these results, a default value of twice the soil half life of a substance is used if no measured data are available to derive this input parameter.

It should be noted that the model assumes there is NO degradation of substance in the 24 hours between application and the first rainfall event. This is because most substances have a soil DT_{50} of more than a few days, thus it is unlikely that significant degradation will occur. However, it is recognized that some substances may dissipate very rapidly, for example as a result of volatilisation or very rapid degradation. In such cases, users should adjust the application amount input parameter (see below) to take account of the amount of substance applied that is likely to be lost via volatilization or other mechanisms during the 24 hours between application and rainfall. **Such an approach should only be used where a significant amount of study data can be presented to justify the proposed reduction in**

the application amount. Based on previous precedent, taking into account uncertainty of the rain free period, the period when dissipation processes can be assumed to occur should be limited to 6 hours not the full 24 hours. In addition, where such an approach is applied, users must also undertake a model run using the full application amount, in order to estimate PECsw resulting from spray drift losses on the day of application. The subsequent risk assessment must take into account the highest predicted concentration from the two model runs.

DT_{50} in sediment (days).

DT_{50} in water (days).

The model requires values for the degradation half life of the substance in both water and sediment. Such values can be derived from water / sediment studies. Comprehensive guidance on deriving such values is provided in the FOCUS Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration (FOCUS, 2006, or the latest version available). However, in the first instance appropriate DT_{50} end-points in sediment and water from the agreed EU peer review and contained in the EFSA Conclusion for the relevant active substance should be used in the model.

Application amount (g/ha) Sub-urban (domestic use). For domestic use products, particularly those that are ‘ready to use’ formulations, details of substance contents in mass per litre may not be on the label nor may there be clear recommendations as to the dose to be applied per unit area. **Model users thus need to pay particular attention to how they derive the application amount used as input to the model and give an argued justification for the value used**.

Fraction of 774.7 m^2 railway track target area actually sprayed. The model has a default worst-case assumption that all of the 774.7 m^2 area of railway track is sprayed by the spray train within one or two days. **This default assumption should not be altered**. Although it is recognized that target weed spraying using, for example, the ‘WeedIt’ technology can significantly reduce the amount of herbicide applied to the track, such technology is only applicable to contact herbicides and, at present, has only very limited use on the rail network.

Runoff attenuation factor applied to leached load from ballast. At present, no experimental study data is available to assess the potential attenuation of substance loads during runoff down the railway embankment side. The model therefore assumes a worst case attenuation factor of 1 (no attenuation). This is very conservative and probably unrealistic and therefore,

providing information is presented to justify the level of attenuation likely to occur, the value can be reduced by the user.

% of applied amount impacting as spray drift (Application to railway tracks from a hand-held sprayer). As with the urban and major road scenarios the model uses a default value of 2.8% derived for a hand held application to a crop < 50 cm high and at a distance of 1 m from the edge of the 'crop' to the start of the water body. **Users should not alter this value unless they wish to examine the potential effect of buffer strips, 'no spray' zones or reduced drift application methods, in which case the alternative values used should be fully justified**.

Fraction of 100m^2 target area spot-sprayed (Application to railway tracks from a hand-held sprayer). The model has a default worst-case assumption that this type of application to railway tracks is applied as a continuous 1m wide swath along the 100 m of track edge adjacent to the railway ditch. However, it is recognized that best practice application encourages the use of spot spraying rather than swath application and, in order to investigate the impact of such methods, users can change the fraction of 100 m^2 target area of track to which spray is applied. **For regulatory applications, any changes to the fraction of track treated must be supported with data to justify the values used**.

3.2 Worksheet "OUTPUT":

The output worksheet provides the user with tabular and graphical information relating to the predicted environmental concentrations (PEC's) in the scenario surface water and groundwater bodies. The acute (maximum) 24 hour concentration in both water and sediment phases of each surface water body is tabulated along with concentration relating to spray drift on the day of application. For groundwater, the peak concentration at the groundwater well and the length of time the PEC is above 0.1 μg L^{-1} are also quantified along with the average annual concentration in the water flux draining out of the railway formation underneath the tracks. Graphs show predicted changes in substance concentrations in water and sediment over time in the surface water bodies and changes in groundwater concentrations over time. Finally, graphs showing the daily rainfall volumes over time and the volumes of water passing through the surface water bodies over time are also provided.

If users wish to calculate time weighted average concentrations they should proceed as follows:

For Surface Water Scenarios. Move to the "Losses_AR" worksheet and copy cells BE16 to BJ89 inclusively, BP16 to BQ89 inclusively, BY16 to BZ89 inclusively and CH16 to CI89 inclusively.

Cells BE16 to 89 provide daily concentrations in the urban stream water phase.

Cells BF16 to 89 provide daily concentrations in the rural major road stream water phase.

Cells BG16 to 89 provide daily concentrations in the domestic usage stream water phase.

Cells BH16 to 89 provide daily concentrations in the urban stream sediment phase.

Cells BI16 to 89 provide daily concentrations in the rural major road stream sediment phase.

Cells BJ16 to 89 provide daily concentrations in the domestic usage stream sediment phase.

Cells BP16 to 89 provide daily concentrations in the urban pond water phase.

Cells BQ16 to 89 provide daily concentrations in the urban pond sediment phase.

Cells BY16 to 89 provide daily concentrations in the Railway ditch water phase resulting from leaching.

Cells BZ16 to 89 provide daily concentrations in the Railway ditch sediment phase resulting from leaching.

Cells CH16 to 89 provide daily concentrations in the Railway ditch water phase resulting from runoff down the embankment side.

Cells CI16 to 89 provide daily concentrations in the Railway ditch sediment phase resulting from runoff down the embankment side.

For Groundwater Scenarios. Move to the "Groundwater model" worksheet and copy cells G5 to 1504 inclusively, CL5 to 1504 and FQ5 to 1504 inclusively.

Cells G5 to 1504 provide daily concentrations in the Sandstone aquifer.

Cells CL5 to 1504 provide daily concentrations in the Chalk aquifer.

Cells FQ5 to 1504 provide daily concentrations in the Limestone aquifer.

Users will need to use the "copy" - "paste special" - "values" functions in MS Excel to copy and paste the relevant values to a new workbook where the data can be manipulated to calculate specific time-weighted average concentrations, as required.

3.3 Worksheet "Domestic_Use_scenario".

This sheet defines the fixed scenario parameters for the Urban catchment as described in Sections 2.1.1 & 2.1.3 of the full Guidance Document (Hollis *et al*, 2017).

3.4 Worksheet “Urban_scenario”.

This sheet defines the fixed scenario parameters for the Urban catchment as described in Sections 2.1.1 & 2.1.3 of the full Guidance Document (Hollis *et al*, 2017).

3.5 Worksheet “Major_scenario”.

This sheet defines the fixed scenario parameters for the Rural Major Road catchment as described in Sections 2.1.1 & 2.1.3 of the full Guidance Document (Hollis *et al*, 2017).

3.6 Worksheet “Railway_scenario”.

This sheet defines the fixed scenario parameters for the Railway catchment as described in Sections 2.1.1 & 2.1.3 of the full Guidance Document (Hollis *et al*, 2017).

3.7 Worksheet “Losses_BR”.

In this sheet, plant interception (a fixed scenario parameter) and spray drift are used to calculate losses before rainfall and to derive the mass of applied substance reaching each hard surface type. The percentage of applied amount of substance impacting as spray drift is an input parameter to the model (see Section 3.1 above) and this amount is adjusted to take into account the fact that, in the urban situation spray drift losses only apply to the length of road running along the east side of the scenario catchment. Spray drift from all other applications in the catchment is assumed to impact on a hard surface and, thus, to be washed off into the catchment drainage network.

3.8 Worksheet “Masses lost per 0.5mm rain”.

This worksheet contains calculations of the ***washoff sub-models*** for each surface type. The calculations are based on a unit area of 0.54 m^2 and are carried out for each daily rainfall event. Each event is separated into 0.5 mm rainfall increments. The worksheet also contains the calculations for routing of wash-off within the surface water catchments.

3.9 Worksheet “Groundwater_model”.

This worksheet is used to calculate dispersion and attenuation of the substance masses leaching to the saturated zone during their transport to the wellhead. Masses arriving at the water table are derived from the relevant cells in the Losses_AR worksheet. Daily concentrations in water arriving at the wellhead are calculated for a period of 1,500 days after the initial arrival of the substance leached from the unsaturated zone, for three aquifer types: Chalk, Limestone and Sandstone.

The model uses a simple analytical solution of the advection dispersion equation corresponding to one dimensional slug injection (Crank, 1956). A separate box is used to derive the model input parameters from the aquifer scenario characteristics. An additional box summarises the assumptions used in the model.

3.10 Worksheet “Railway_surface_water”:

This worksheet is used to calculate dispersion and attenuation of the substance masses that have leached into the saturated zone during their transport to the adjacent surface water ditch. Masses arriving at each 1m section of the water table below the railway are derived from the relevant cells in the Losses_AR worksheet. For each 1m section, daily concentrations in water arriving at the wellhead are calculated for a period of 365 days after the initial arrival of the substance leached from the unsaturated zone.

The model uses a simple analytical solution of the advection dispersion equation corresponding to one dimensional slug injection (Crank, 1956). A separate box is used to derive the model input parameters from the chalk aquifer characteristics in the “Railway_scenario” worksheet. An additional box summarises the assumptions used in the model.

3.11 Worksheet “Losses_AR”:

In this worksheet, all the losses during and after rainfall are calculated for each scenario. For surface water scenarios, the sheet is separated into calculations for: Rainfall volumes; Runoff volumes; Runoff from each surface as a % of total runoff from the scenario; Volumes of water flowing through the water bodies per rainfall event; Depth of water in the stream scenarios per rainfall event; Total mass of substance lost per rainfall event; Accumulated loss of substance as a % of the applied mass; Total mass of substance entering the water body per rainfall event; Input mass of substance to the water phase of each water body per rainfall event; Input mass of substance to the sediment phase of each water body per rainfall event; Residual mass of substance in the water phase of the pond per rainfall event; Residual mass of substance in the sediment phase of each water body per rainfall event; Final mass of substance in the water phase of each water body per rainfall event; Final mass of substance in the sediment phase of each water body per rainfall event; Concentration of substance in the water phase of each water body per rainfall event; Concentration of substance in the sediment phase of each water body per rainfall event.

For the Groundwater scenario, the sheet is separated into calculations for: Accumulated daily rainfall; Accumulated substance mass lost from the railway ballast layer; Daily substance mass lost from the railway ballast layer; Daily attenuated substance mass reaching the groundwater surface from the unsaturated zone of a Chalk, Limestone and Sandstone aquifer.

Separate ‘boxes’ are used to calculate the number of 0.54 m^2 ‘blocks’ for each surface type in each scenario, based on the fixed scenario parameters, the fraction of input to the sediment and water phases of each water body and the unsaturated zone travel times for each Aquifer type. The sheet also includes fixed scenario parameter values relating to: The % runoff of rainfall from each surface type present in the surface water catchments and the physical characteristics of the stream and pond water bodies.

3.12 Regulatory Context for Use of the Model

It is clear from the work presented and discussed in this report that the main use for which the model has been developed is as a first-tier estimation of substance concentrations in surface and ground waters in the UK, resulting from product use in professional amenity and amateur home garden situations on ‘hard surfaces’, according to existing UK and EU legislation on Plant Protection Products. It is within this context that the CRD welcomes the submission of modelling exposure data from applicant companies, as part of their regulatory dossiers for UK approval of such substance products in the professional amenity and amateur home garden situations which are proposed for use on hard surfaces not intended to bear vegetation. In general, if applicant companies wish to use the model outside of this context, the onus rests with the company to demonstrate clearly the suitability of the model and to justify its use in the proposed new situation. Included here would be possible extensions of use, such as – pesticides other than herbicides, approval applications outside the UK, application types other than spraying.

The model produces estimated exposure concentrations (Predicted Environmental Concentrations, PEC) for surface and ground waters. In the case of the PEC values for surface water, these should be compared with the appropriate ecotoxicological endpoints to produce the toxicity:exposure ratios (TER) values for use in the tiered risk assessment process for non-target organisms in the aquatic surface water environment. Applicants are invited to seek further guidance on the conduct of the risk assessment from the CRD website.

In the case of PEC values for groundwater, these should be compared with the EU pesticide threshold concentration for all groundwaters of 0.1 $\mu g\ L^{-1}$ (i.e. the maximum admissible concentration for drinking water in the EU). For more guidance on the issue of regulatory assessment of pesticides in groundwater, readers are referred to the various guidance documents associated with the EU Regulation 1107/2009.

The model described in this report produces first-tier exposure estimations. Where first tier assessments lead to a failure of risk assessment, Applicants should initially consult the HardSPEC guidance and the CRD website for guidance on potential refinements to HardSPEC assessments and are encouraged to contact CRD to discuss their suitability.

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