Research Article

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Effects of soil redistribution by tillage on subsequent transport of pesticide to subsurface drains

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Abstract

BACKGROUND: Tillage operations will change the distribution in soil for any pesticide residues still present from earlier applications. This redistributive effect of tillage has been neglected in the study of pesticide leaching behavior. This study reviews the literature to characterize this redistributive effect for different tillage operations and uses a pesticide leaching model to investigate the impact of redistribution on pesticide transport to subsurface drains which is a significant input route to surface water bodies.

RESULTS: Inversion ploughing moves the majority of any residues of pesticide present at or near the soil surface into the bottom two-thirds of the plough layer, whereas non-inversion ploughing has only a limited redistributive effect. Incorporating this redistributive effect into model simulations resulted in large changes (typically 5–10-fold difference) in both the maximum concentration and total mass of pesticide transported to drains over the winter following cultivation. More intense cultivation decreased subsequent leaching for relatively mobile compounds (Koc ≤1000 mL g^{-1}), but increased it for strongly sorbed pesticides (Koc ≥2000 mL g^{-1}).

CONCLUSION: The redistributive effect of soil tillage on pesticide residues can have a large effect on subsequent transport to subsurface drains. This effect has been neglected in the literature. Field research is required to validate the model simulations presented here, and consideration should be given as to whether the effect needs to be included within risk assessment procedures.

Supporting information may be found in the online version of this article.

Keywords: cultivation; plough; leaching; MACRO; model; risk assessment

1 INTRODUCTION

A thorough understanding of pesticide fate and behavior under a range of both environmental conditions and agronomic practices is essential to ensure safe use of new and existing plant protection products. Pesticide properties, formulation type, soil type, soil drainage status, and weather are all known to influence transport of pesticides in soil.[1,2] There are multiple studies, many from the last two decades of the 20th century, that compare pesticide leaching under different tillage regimes; these focus on the effects of modified soil properties associated with conventional tillage (normally involving inversion ploughing), conservation (or minimum) tillage, and no- (or zero-) till.[3] Typical experiments have followed the fate of pesticides applied to plots that have previously been managed with different tillage practices. Soils subjected to a no-till regime often exhibit higher pesticide concentrations leaching to depth and/or to subsurface drains than the same soil under conventional tillage. This observation has been attributed to preferential flow through the more extensive network of structural and biological macropores that can develop under no-till conditions.[4–7] Nevertheless, there is variability in the literature and other studies have reported no significant effect of tillage system on pesticide leaching through soil.[8,9]

As well as influencing soil properties, tillage operations will redistribute solutes and other material such as crop residues that are present in the upper layers of soil prior to cultivation. This physical redistribution is likely to modify subsequent leaching behavior, so it is surprising that this effect has been ignored almost completely within the pesticide literature to date. Experiments to investigate this effect would need to follow fate of pesticides applied to plots with identical hydraulic properties with and without post-treatment tillage of the soil. Berger *et al.*[10] investigated the distribution and persistence of surface-applied

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trifluralin in soil following applications in three successive seasons with incorporation using either inversion ploughing plus harrowing or with harrowing alone. There was no impact of the cultivation regime on persistence, but larger residues were found to 30-cm depth following inversion ploughing plus harrowing compared to soil that was only harrowed. Although trifluralin residues in soil were not detectable below the plough layer, the authors inferred a greater risk of leaching with the use of inversion ploughing. A review by Alletto *et al.*[3] identified that pesticide incorporation into soil by tillage significantly reduced losses by runoff in comparison to pesticide left at or close to the soil surface, and postulated that this technique could lead to an increase in losses by leaching. Conversely, Jones *et al.*[11] stated that pesticide incorporation into soil was found to have no effect on transport of isoproturon to drains in a single plot experiment on a heavy clay soil, but did not provide further details.

Thus, there is a gap in knowledge relating to whether physical redistribution of any pesticide residues in soil as a result of soil tillage operations will affect subsequent leaching behavior. Physical redistribution will be relevant particularly to those pesticides that are likely to persist in soil to the start of the agronomic season that follows application. Many fungicides, for example, may be applied near the end of the preceding crop cycle and several groups including the triazoles are known to be relatively persistent in soil. Any modification of leaching behavior *via* physical redistribution will also play a significant role in the fate of pesticides which are deliberately incorporated, for example to restrict losses *via* volatilization or surface runoff.

In this work we first present a review of the relevant literature to determine the extent and pattern of pesticide redistribution under different cultivation operations. Results from this review are then incorporated into the mathematical model MACRO[12] to investigate the effect of physical redistribution on subsequent leaching of pesticide to drains. A standard modelling scenario that is currently operational in EU regulatory practice for assessing pesticide transport to surface water bodies[13] is used as the basis for this modelling exercise.

2 REVIEW OF EXPERIMENTAL STUDIES INTO THE REDISTRIBUTIVE EFFECT OF DIFFERENT SOIL TILLAGE OPERATIONS

2.1 Experimental approach

A literature search identified eight journal articles that report studies to characterize the redistributive effect of different soil tillage operations. Key features of these studies are summarized in Table 1. Most studies into redistribution during tillage operations added physical tracer either to the soil surface or uniformly at specified depths within the cultivation zone. These physical tracers differed in size (ranging from 1 to 6 mm) and included ceramic spheres,[14,15] aluminum cubes,[16,17] and plastic beads.[18] Most studies considered that physical tracers are good substitutes for incorporated granule or surface spray, although Logsdon[19] argues that larger tracers may not be representative of smaller aggregates/single grain particles unless the soil is highly structured. Allmaras *et al.*[14] found that patterns of redistribution were similar when they compared ceramic tracers and oat seeds. Spokas *et al.*[18] conducted initial experiments using beads of two different diameters (3 mm and 6 mm) and concluded that bead size did not affect the position of the beads in post-tillage profiles. Soriano *et al.*[20] also observed no differences in the distribution of seeds with differing sizes after tillage.

Studies using physical tracers recovered them either through soil core sampling[14,15] or through field soil excavation.[18,21] Although field excavation is a labor-intensive process, it can achieve high recovery rates of beads (>90%) and accurate accounting of soil translocation from tillage.[18] This method is more effective than soil core sampling, with the latter resulting in a wider range of tracer recovery rates. For example, recovery rates of tracers after primary tillage were 80 ± 9.6% SE for chisel plough and 75 ± 7.6% SE for moldboard plough.[14]

Another method used to investigate soil redistribution involves the removal of a section of soil at a specified depth and replacement with dyed sand or soil. Logsdon[19] used yellow and blue painted limestone placed at the top (0–10 cm) and bottom (20–30 cm) of a trench, respectively. Similarly, Scanlan and Davies[22] used blue and green synthetic soil created by mixing a color-coated sand with kaolinitic clay. One limitation of this technique is that the colored sand replacement may behave differently to original field soil due to differing physical properties. To account for this, dyed sand and soil was mixed at a ratio of 1:10 to produce a soil that matched the bulk density and texture of field soil as closely as possible.[22]

Redistribution of dyed sand or soil was visualized by excavating the soil and capturing a series of digital images of each vertical slice through the soil profile.[22,23] Image processing involved altering the image saturation, classifying pixels into groups and constructing three-dimensional data. Logsdon[19] used an alternative method where an incremental sampler was used to extract subsamples of soil to 30-cm depth. One constraint to this imaging approach is that the data are representative for a relatively small cross-section of soil. This is especially important for cultivation implements such as the rotary spader as results will only show part of the full rotation of the spader.[22]

2.2 Tillage operations investigated

The cultivation techniques that have been compared within the eight journal articles include both primary and secondary tillage operations (Table 2 and Table 3) which together make up most conventional tillage systems. Primary cultivation usually consists of inverting the soil with a moldboard plough[24] or the use of non-inversion ploughing such as with a chisel plough. Six articles included moldboard plough within the study, whilst four included chisel plough (Table 2). Secondary cultivation refers to the use of a cultivator to produce a seedbed for drilling.[24] Five articles included the effects of secondary tillage operations. Allmaras *et al.*[14] looked at incorporation in a sequential tillage operation by applying the tracers after primary tillage (green spheres) and secondary tillage (red spheres). Staricka *et al.*[15] combined both moldboard plough and chisel plough with secondary tillage comprising a tandem disk, as is common in conventional tillage.

A broad spectrum of soil texture was explored within the literature (Table 1). Milkevych *et al.*[17] compared the effect of tillage in three soil types comprising a coarse sand, a loamy sand and a sandy loam. A few studies accounted for operational speed[18,19,23] [18,19,23] and working depth[18,23] of the cultivation practices. Scanlan and Davies[22] quantified soil mixing as well as redistribution from four different tillage practices (disc harrow and deep ripping, disc plough, moldboard plough and rotary spader).

2.3 Findings for redistributive effects of primary cultivation methods

Results from the five studies that investigated the redistributive effects of moldboard ploughing show similar overall patterns,

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Table 1. Approaches used in literature investigating the redistributive effects of different cultivation practices, and other factors relating to tillage techniques that were considered to have an effect. MP = Moldboard plough, CP = Chisel plough, H = Harrowing, TD = Tandem disc, DP = Disc plough, DHDR = Disk harrow with deep ripping, RS = Rotary spader, SC = Sweep cultivation

Reference	Experimental design	Tillage practices compared	Tracer application	Tracer size	Sampling/analysis process	Soil texture
Staricka *et al.*[15]	Field experiment, strip plot design with four replications	CP + TD *vs* MP + TD	Ceramic spheres and seeds of foxtail millet sprayed with fluorescent red paint, surface applied. Soybean and oat grown in strips.	Seeds - 1 to 2 mm in diameter with a mass of 2.55 mg. Ceramic spheres - 1 to 3 mm in diameter mass of 1.48 mg	Soil cores taken – 18 mm in diameter, taken to a depth of 50	Not specified
Allmaras *et al.*[14]	Field experiment	MP *vs* CP *vs* H MP + H *vs* CP + H	Green and red ceramic spheres and oat residue broadcast uniformly by hand at application rate of 2.1 spheres cm^{-2}	1–3 mm	30 cm long core obtained from 5 × 5 m area, air dried and weighed. Ceramic spheres counted	Silt loam (fine silt over sandy)
Spokas *et al.*[18]	Field experiments, 5–10 replicates for each tillage method	MP *vs* CP *vs* 10 others	Plastic tracer beads buried manually in soil. Burial locations 8 cm diameter hole created with soil bucket auger to 25 cm depth. 12 different plastic bead colors buried at 1 cm intervals to 12 cm and then 15, 17, 20 and 25 cm (below depth of tillage). 30 beads at each depth (bead density of 6000 beads m^{-2}) placed randomly in the intended path of tillage implement. For residue management and strip-tillage methods, beads only buried in crop row where soil disturbance occurred	6 mm diameter	Field soil excavation *in situ*. Exact placement of each bead recorded – both horizontal and vertical translocation. Beads found on surface flagged and position recorded	Silty clay loam
Milkevych *et al.*[17]	Four outdoor soil bins (40 × 2.7 × 1.5 m), each divided into three plots with width of 0.7 m.	SC	Aluminum color-coded cubes (total of 33) inserted into soil in a grid at 0, 5 and 10 cm depth placed up to 25 cm distance from central sweep line. Coordinates recorded	15 × 15 mm	The local soil cross-sectional disturbance was measured using a 390 mm wide profile meter consisting of 130 free-dropping wooden pins Loose soil in the furrow excavated and placed the profile meter across the furrow 36 sections with 12 per bin. Profiles obtained used to analyze characteristics of the local soil disturbance	Coarse sand, loamy sand and sandy loam

Table 1. Continued

Reference	Experimental design	Tillage practices compared	Tracer application	Tracer size	Sampling/analysis process	Soil texture
Cousens and Moss[16]	A matrix model set up from a single field experiment and published works	MP	Aluminum cubes	15 × 15 mm		Sandy loam
Scanlan and Davies[22]	Field experiment over two sites with tillage treatments arranged as parallel strips	MP *vs* RS *vs* DP *vs* DHDR	Prior to treatments, synthetic colored soil installed in narrow trenches 100 cm wide, 10 cm long and 30 cm deep at two sites Blue soil installed at 0–10 cm depth and green soil at 20–30 cm depth. The synthetic soil was created by mixing a color-coated sand with kaolinitic-clay at a ratio of 10:1 by weight	N/A	Series of digital images for all tillage treatments and sites to capture 3D distribution of colored soil tracer. At each site a pit dug 100 cm deep, 200 cm wide by 200 cm long with a mini-excavator and photographed pit face. Images processed – saturation altered, then classified pixels into groups. 3- dimensional data constructed from this using the rgl package in R	Sand
Ucgul *et al.*[23]	1/3 scale moldboard plough tested in soil bin 90 (L) x 50 (W) x 17 (D) cm. Topsoil burial simulated using a discrete element method	MP	Trench prepared across path of plough 300 (L) x 20 (W) x 40 (D) cm and filled with blue colored sand	N/A	Four vertical excavations at 25 cm increments across the direction of travel and digital photos of each slice taken. Digitally analyzed using MATLAB 2015 determine pixel locations of blue colored sand particles.	Sandy loam soil
Logsdon[19]	Field experiment	CP	Painted calcium carbonate (limestone) Trench prepared across the path of plough (122 cm long 10 cm depth and 13 cm) filled with painted calcium carbonate (limestone) Blue limestone - 5.51 kg per trench, placed into trenches 122 (L) x 13 (W) x 10 (D) cm. Yellow limestone - 6.89 kg per site, surface applied to an area 122 (L) x 56 (W) cm	1–8 mm diameter particles	Incremental sampler used to extract sub-samples to 30 cm depth. Samples subdivided into 2.5 cm incremental depth units. Yellow and blue tracers were hand-picked from each sample and weighed.	Not specified

Table 2. Primary cultivation techniques investigated in experimental redistribution studies, including details on working depth and machine specification

Reference	Working depth	Name/details
Moldboard plough (MP)		
Scanlan and Davies[22]	30 cm	Kvernerland MP fitted with skimmers
Staricka *et al.*[15]	30 cm	Five 46 cm bottoms for a working width of 2.3 m
Cousens and Moss[16]	Not specified	Not specified
Allmaras *et al.*[14]	25 cm	Three 41 cm shares
Spokas *et al.*[18]	24 cm	Case 500
Ucgul *et al.*[23]	30 cm	5 km hr^{-1} speed. 3 furrow commercial plough with skimmers
Chisel plough (CP)		
Allmaras *et al.*[14]	15 cm	Frame 2.74 m wide with 10 shanks set 30 cm apart
Staricka *et al.*[15]	10 cm	8 cm wide, concave- twisted shanks spaced 30 cm apart and a working width of 4.6 m
Logsdon, 2013[19]	12 cm	Twisted shank chisel plough - shank spacing was 0.38 m apart, with a maximum depth of 0.2 m right at the shank (less between the shanks). mean speed was 1.8 m s^{-1}
Spokas *et al.*[18]	23 cm	John Deere 610
Disk plough		
Scanlan and Davies[22]	30 cm	McCormick International A1-41 4-disc plough fitted with 65 cm discs
Spokas *et al.*[18]	11 cm	John Deere 115
Paraplough		
Spokas *et al.*[18]	25 cm	Howard
Rotary plough		
Scanlan and Davies[22]	25 cm	Farmax 4.5 m trailed rotary spader

Table 3. Secondary cultivation techniques investigated in experimental redistribution studies, including details on working depth and machine specification

Reference	Tillage practice	Working depth	Name/details
Allmaras *et al.*[14]	Shank-type cultivator with a trailing harrow	<11 cm	Cultivator frame was 3.35 m wide with shanks mounted on three ranks. Shank spacing on each rank was 45 cm with mounted narrow chisel-point shovels 6 cm wide and 30 cm long
Staricka *et al.*[15]	Tandem disk	8 cm	5.9 m wide tandem disk with 56 cm con- cave disk blades on an 18-cm spacing
Scanlan and Davies[22]	Disc harrow followed by deep ripper	30 cm	Applied in two operations. International 3–3 disc harrow fitted with 55 cm discs
Spokas *et al.*[18]	Field cultivator	12 cm	WilRich 2500
Spokas *et al.*[18]	Rotary hoe	7 cm	John Deere 400
Milkevych *et al.*[17]	Sweep cultivator	10 cm	Width of 180 mm; sweep angle, 80°, and rake angle, 15° (we refer to (Fielke and Riley, 1991) for detailed definition of sweep geometry). The sweep, together with a 46 mm wide shank, was mounted on a toolbar

but also some differences in the final location of tracers with depths (Fig. 1). All studies measured the smallest proportion of residues in the 0–10 cm layer (4–22% of applied tracer). Scanlan and Davies[22] and Allmaras *et al.*[14] found similar patterns in deeper soil layers with the majority of the tracers recovered from 10–20 cm depths (58 and 62%, respectively), whilst others found the largest proportion of tracers had been redistributed to the 20–30 cm soil layer (39–53% of applied tracer[15,16,23]). Results from all studies are expressed on a common depth increment of 5-cm in Fig. 1. However, it is likely that the variation in residues with depth is underestimated in those studies with the largest sampling increments of 5 to 10 cm layers.[15,22,23]

Literature on the redistributive effects of chisel plough show greater consistency (Fig. 2) than for moldboard plough. In all cases, the largest proportion of the tracer was recovered from the top 0 to 5 cm of soil (47–88% of applied tracer) and there was very little redistribution below a depth of 15 cm (maximum 6% of applied tracer). Despite using very different methods, Allmaras *et al.*[14] and Logsdon[19] both used a small sampling increment of 2.0 or 2.5 cm in the topsoil layer and obtained similar results for the redistributive effects of a chisel plough. One interesting observation is that the chisel plough study with the deepest working depth (23 cm[18]) did not result in the deepest redistribution of soil.

The extent of mechanical soil redistribution is usually related directly to the harshness of the tillage operation.[25] Overall, studies confirm a larger vertical redistributive effect on soil with moldboard plough compared to non-inversion tillage practices. This

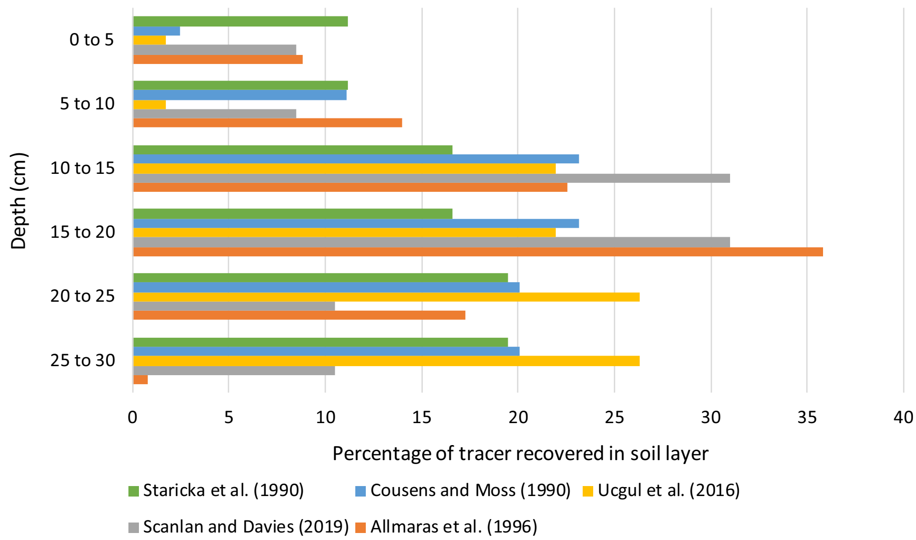

Figure 1. Percentage of tracers that were applied to the top 0–10 cm of soil and that were subsequently recovered from soil layers down to 30 cm after inversion ploughing with a moldboard plough. All studies were without any secondary cultivation apart from Staricka *et al.*[15] which used a tandem disc after the moldboard plough.

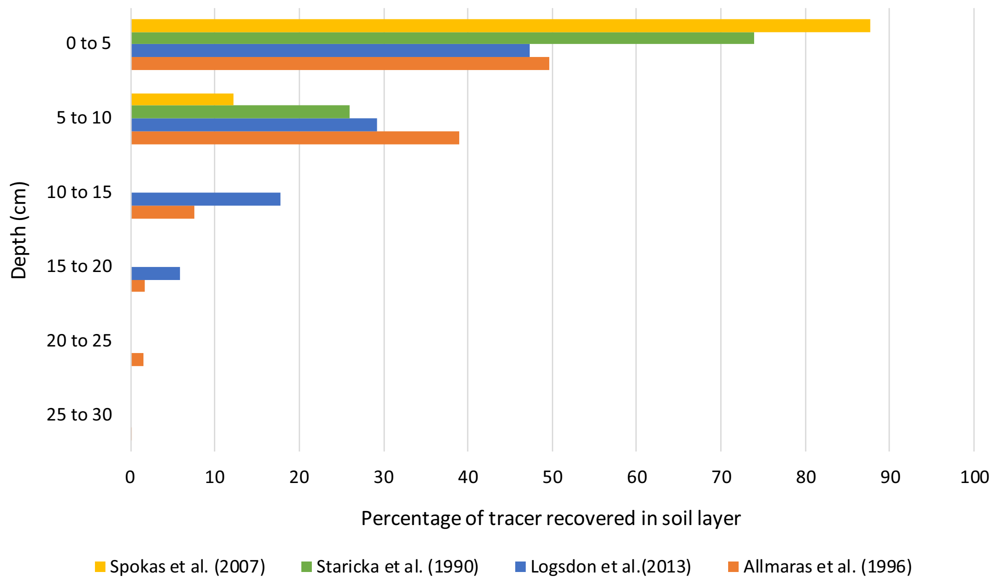

Figure 2. Percentage of tracers that were applied to the top 0–10 cm of soil and that were subsequently recovered from soil layers down to 30 cm after non-inversion ploughing with a chisel plough. All studies were without any secondary cultivation apart from Staricka *et al.*[15] which used a tandem disc after the chisel plough.

relates both to the depth of penetration and the intensity of soil redistribution (Fig. 1 and Fig. 2). For example, Allmaras *et al.*[14] investigated the distribution of crop residue and ceramic spheres in the tilled layer after both moldboard plough to a depth of 25–30 cm and chisel plough to a depth of 15 cm and found significant differences. Soil cores extracted after primary tillage had weighted mean depths for ceramic spheres of 12.7 $\pm$ 1.3 cm after moldboard ploughing and 4.4 $\pm$ 1.4 cm after chisel ploughing. Most of the surface soil is buried during inversion ploughing, meaning that any pesticide residue previously residing at or near the soil surface will be incorporated to a large extent towards the bottom of the plough working depth. Only 4% of recovered ceramic tracers were found in the top 4 cm of the soil after moldboard ploughing compared to 48% found after chisel ploughing.[15] Pareja *et al.*[26] found 85% of all weed seeds were in the upper 5 cm of soil in reduced tillage systems, but only 28% after inversion (moldboard) ploughing.

2.4 Findings for redistributive effects of secondary cultivation methods

When harrowing was undertaken after moldboard ploughing, it was found to have no significant effect on the distribution of green spheres used as a tracer in soil.[14] Red spheres applied to the surface after moldboard ploughing and before harrowing were not incorporated as deeply into the soil as those in a treatment with harrowing of unploughed soil. It was concluded that the presence of freshly buried residue reduced the incorporation of the red spheres into deeper layers.[14] This is supported by

Staricka *et al.*[15] who found that secondary tillage did not significantly change the pattern of seed burial when used in conjunction with moldboard or chisel ploughing treatments; the authors suggested that this was related to the working depth of <10 cm for the tandem disk that was investigated. A recent study confirmed a limited redistributive effect for disk harrow followed by deep ripping, with only 10% of dyed soil from the top 10 cm translocated to greater depths.[22] Whilst the three-dimensional model employed by Scanlan and Davies[22] is a very effective method for visualizing the effect of tillage on soil redistribution, one limitation of their study is that the quantification is at a coarse resolution and only reveals redistribution patterns at 10-cm increments.

2.5 Influence of other factors

In addition to vertical redistribution of soil and associated residues during tillage, several studies focus on the lateral and longitudinal translocation of soil. Using tracers at the soil surface placed at three different depths (0, 5 and 10 cm), Milkevych *et al.*[17] found that vertical displacement was 0–3 cm for tracers placed at the soil surface, 0–5.5 cm for tracers placed at 5-cm depth, and 0–4.4 cm for tracers placed at 10 cm depth. Vertical displacement was smallest in terms of magnitude, compared to lateral and longitudinal translocation. The study also found that vertical displacement was greatest at the sides of the plough, rather than at the center.

Forward travel speed of moldboard ploughing is likely to have an effect on soil redistribution during ploughing. Ucgul *et al.*[23] carried out a field experiment using blue colored sand and calculated the percentage of surface soil burial by moldboard ploughing to validate a model. Topsoil burial was then simulated for moldboard ploughing to 30 cm depth undertaken at speeds of 5, 7.5 and 10 km hr^{-1}. Soil ploughed at 10 km hr^{-1} was predicted to have the least burial of surface soil; thus 37.4% of surface soil was retained in the upper 10 cm at 10 km hr^{-1} compared to 12.1% at 5 km hr^{-1}, and only 7.3% of surface soil was redistributed to the 20–30 cm soil layer at 10 km hr^{-1} compared to 35.3% at 5 km hr^{-1}.

Despite a large amount of vertical soil redistribution to other layers within the plough layer, Scanlan and Davies[22] found that the degree of mixing within that soil was minimal. The soil mixing that occurred between three layers (depths 0–10, 10–20 and 20–30 cm) was quantified using a mixing index. Mixing indices were low after all tillage treatments, ranging from 0.04 to 0.12 where 0 represents complete segregation and 1 represents perfect mixing. Moldboard ploughing resulted in the least amount of mixing. This cultivation technique rotated and redistributed soil which remained in distinct seams or patches.[22] Further experimental studies that examine the extent of mixing within the soil horizons are needed for different soil types.

3 MODELLING TO INVESTIGATE THE EFFECT OF REDISTRIBUTION OF PESTICIDE RESIDUES ON LEACHING TO DRAINS

3.1 Model scenario and parameterization

The preferential flow model MACRO 5.2 was used to investigate the effect of physical redistribution of pesticide residues on subsequent leaching to subsurface drains. MACRO simulates the influence of preferential flow on transport of solutes including pesticides by dividing the soil into micropore and macropore domains. The processes simulated by the model are outlined in the Supplementary Material, and the governing equations are comprehensively described elsewhere.[12,27] The MACRO model has been evaluated extensively under European conditions.[28–31]

Aquatic risk assessment for pesticides in Europe requires the calculation of predicted environmental concentrations in surface water following entry *via* spray drift, surface runoff and drainflow. Standard scenarios have been defined that capture the variability in soils, cropping and weather conditions across the European Union, and these are used as input to mathematical models to estimate concentrations in water. For pesticide transport to surface water *via* drainflow, the MACRO model is used in combination with a set of six standard scenarios to estimate predicted environmental concentrations.[13] Scenario D2 is particularly vulnerable, representing a worst-case soil type for drained land in Europe coupled with vulnerable temperature and water regime.[13] The D2 scenario is based on an impermeable, heavy clay soil with field drains representative of the Brimstone Farm experimental site in central England. The soil is a pelostagnogley with extensive structural cracking that makes it particularly vulnerable to rapid vertical transport of pesticides *via* macropore flow.[32] At the time the scenarios were defined, D2 was considered to cover 0.8% of the agricultural land in the EU and to lie at the extreme end (98.8th percentile) of vulnerability for transport of pesticides to drains.[13] Modelling based on the D2 soil will thus exaggerate any impact of macropore flow on the redistributive effect investigated here compared to more moderate soils across the EU. The FOCUS scenarios were developed to represent soils subjected to conventional tillage,[13] which can be broadly interpreted as inversion (*e.g.* moldboard) ploughing followed by secondary cultivation (*e.g.* harrowing) to produce the seedbed. Although there is increasing use of reduced or no-till practices in the EU,[33] conventional tillage represents the most common cultivation practice across the EU. Despite this, the effects of physical redistribution of pesticide residues in soil during cultivation are not included within the standard FOCUS surface water scenarios.[13]

The D2 surface water scenario was run using MACRO 5.2. The standard D2 scenario parameters[13] were used for all simulations and included the D2 weather data and cultivation of a winter cereal crop. The model was then used to evaluate the effect of redistribution due to various tillage treatments (moldboard plough + harrowing, chisel plough + harrowing, and harrowing alone) on the transport of 21 hypothetical pesticides with varying Koc and DT50. The simulations were set up to consider a pesticide that had been applied prior to cultivation (*i.e.* carryover from the preceding season). First, simulations were run from 1st January 1980 to 30th September 1986 to obtain soil temperature and moisture content at the end of the simulation for each numerical layer within the model. This duration is considered necessary to provide a sufficient model warm-up period to allow conditions to reach steady state.[13] Subsequent simulations were run from 1 October 1986 (with pesticide application occurring on this date) using the previously obtained soil temperature and moisture content as starting values within the model and with different patterns of pesticide specified to imitate the effects of different cultivation practices. Simulations were run until 31st May 1987 to capture pesticide leaching behavior across the full winter drainflow season. This approach of simulating pesticide transport across a single year mirrored regulatory practice in place at the time. Modelling of different weather years would change predictions for both the maximum concentrations and total loadings of pesticides in drainflow, but would not be expected to have a marked effect on the relative impact of physical redistribution of residues during tillage on subsequent transport behavior.

For all simulations, initial pesticide concentrations in soil summed to 100 mg m^{-2} (equivalent to 1000 g active substance ha^{-1}), but with different spatial distribution patterns created down the soil profile to represent the redistributive effect of soil cultivation on pesticide residues in soil (Table 4). Although it is possible to simulate different intensities of tillage in MACRO and their impact on intrinsic soil properties (*e.g.* bulk density and macropore size distribution), this additional effect of tillage was not included here because we specifically sought to isolate any effects of physical redistribution of pesticide residues during tillage operations on subsequent transport behavior. For comparison, simulations were also run with initial conditions where all pesticide was present in the upper soil layer (0.3 cm in depth; zero cultivation), and with pesticide uniformly mixed through the upper 20 cm of soil (uniform incorporation).

Within each treatment, pesticides were simulated with all combinations of varying Koc (20, 200, 500, 1000, 1500, 2000, and 5000 mL g^{-1}) and DT50 (10, 50, and 200 days). Freundlich partition coefficients were calculated from Koc values using the organic carbon content of the respective soil horizon and the Freundlich exponent was set to a default value of 0.9.[13] Degradation in soil was assumed to be influenced by soil temperature and moisture using the current default assumptions utilized in EU regulatory modelling as recommended by FOCUS[13] and EFSA.[34] The effect of different tillage practices (*i.e.* different patterns of residue redistribution) on pesticide transport to drains was assessed by calculating the maximum daily concentration of pesticide in drainflow and the total loss of pesticide to drains between 1st October 1986 and 31st May 1987.

3.2 Results and discussion

For any given cultivation treatment, Koc was the primary influence on both maximum concentration (Fig. 3; Table S1 in the Supporting Information) and cumulative seasonal loss (Fig. 4; Supporting Information Table S2) of pesticide in drainflow, whilst DT50 was a secondary influence. For example, for any given cultivation treatment, the maximum concentration in drainflow decreased by two to three orders of magnitude as Koc increased from 20 to 2000 mL g^{-1}, whereas it increased by less than one order of magnitude as DT50 increased from 10 to 200 days.

Comparison of simulations for different cultivation treatments for any given combination of Koc and DT50 shows that in every case cultivation had a large effect on the overall transport to drains. Typically, there was a 5 to 10-fold difference in maximum concentration (Fig. 3) and seasonal loss (Fig. 4) between cultivation treatments, although at the extremes the maximum concentrations in drainflow differed by more than an order of magnitude. There was a systematic pattern in the influence of cultivation treatment on pesticide transport to drains that was similar for both maximum concentration in drainflow and seasonal loss to drains. Thus, the surface application yielded the largest transport to drains for all values of Koc up to 1000 mL g^{-1} for the maximum concentration in drainflow and up to 1500 mL g^{-1} for the seasonal loss. Conversely, moldboard plough + harrow yielded the least overall transport to drains for pesticides with Koc up to 1000 mL g^{-1} (Fig. 4), and uniform incorporation resulted in the smallest maximum concentrations in drainflow (Fig. 3). For pesticides with Koc values up to 500 mL g^{-1}, the rank ordering of cultivation treatment from greatest to least transport to drains was: surface application > harrow > chisel plough + harrow > uniform incorporation ≈ moldboard plough + harrow. For the simulations with Koc of 2000 mL g^{-1}, there was a complete reversal of the ordering of cultivation treatment with surface application yielding the least transport to drains, followed by harrow, chisel plough + harrow, and with uniform incorporation and moldboard plough + harrow yielding the greatest transport.

The results presented in Figs 3 and 4 indicate that two competing processes influenced the simulation of pesticide transport within the model. First, there was a reduction in transport to drains when part of the pesticide was located away from the near-surface layers of soil at the start of the simulation (1st October 1986). It is known that preferential flow is frequently initiated in these upper soil layers,[35] so that pesticide residing in the soil matrix at greater depth could be protected from such rapid transport. Such an effect has been demonstrated experimentally for shallow incorporation of phosphorus fertilizer into soil.[36,37] Hence, any cultivation that reduces availability of pesticide near the soil surface for rapid transport *via* preferential flow can be expected to reduce pesticide transport to drains. The second process involved mass movement of pesticide during cultivation, whereby pesticide was instantaneously moved with the soil to deeper depths than would otherwise be the case. Surface availability appeared to be dominant within the model when simulating the transport of relatively mobile compounds (Koc ≤1000 mL g^{-1}). Conversely, the mass movement became increasingly important for higher Koc pesticides that would otherwise be relatively immobile within soil, and this was the dominant process for compounds with Koc ≥2000 mL g^{-1}. There was no fixed pattern to the effect of cultivation treatment for compounds with Koc between 1000 and 2000 mL g^{-1} so that the cultivation

Table 4. Areic mass of pesticide (mg m^{-2}) used as starting values (1st October 1986) for simulation of different cultivation treatments within MACRO. Values for different combinations of ploughing and harrowing are adapted from Allmaras *et al.*[14]

Depth (cm)	Moldboard plough and harrowing	Chisel plough and harrowing	Harrowing	Surface application	Uniform incorporation
0–2	4.20	24.98	48.13	100	10
2–4	4.74	37.59	43.68	0	10
4–6	7.07	19.35	6.97	0	10
6–8	10.60	10.10	1.22	0	10
8–10	18.88	3.94	0.00	0	10
10–11	26.97	0.45	0.00	0	10
12–14	17.11	0.61	0.00	0	10
14–16	8.54	0.71	0.00	0	10
16–18	1.46	0.94	0.00	0	10
18–20	0.42	1.33	0.00	0	10

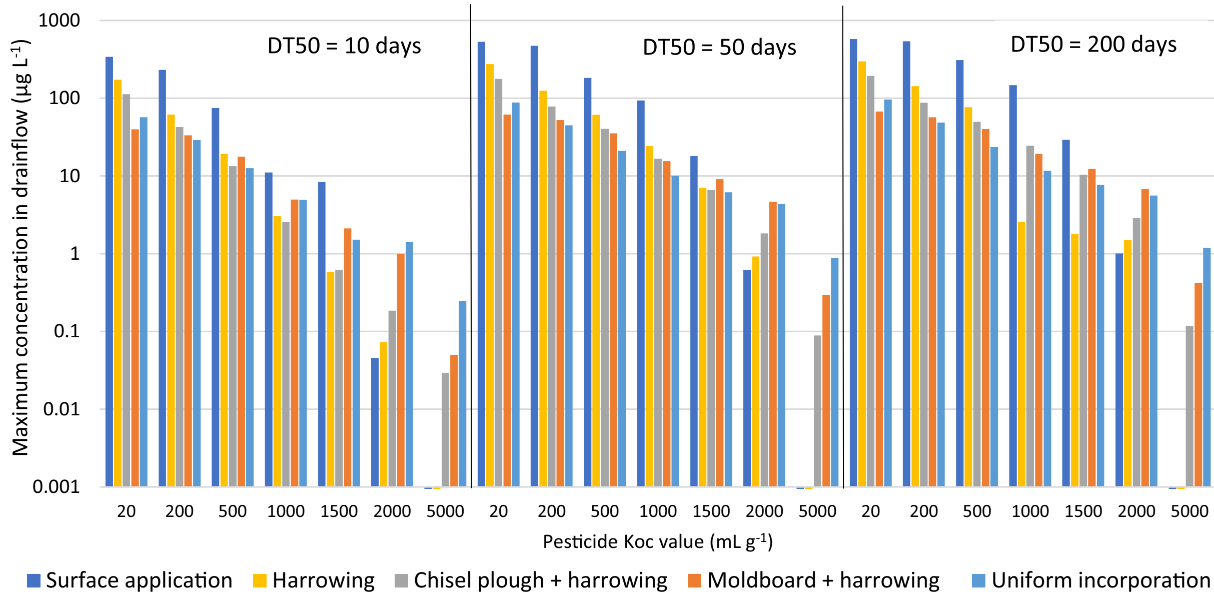

Figure 3. Maximum pesticide concentration in drainflow (µg L^{-1}) simulated using MACRO 5.2 for different patterns of redistribution of pesticide residues in soil due to cultivation. Five cultivations patterns were simulated for pesticides with all combinations of Koc (20 to 5000 mL g^{-1}) and DT50 (10, 50 or 200 days). Results for pesticides with Koc = 5000 mL g^{-1} based on surface application and harrowing were < 0.001 µg L^{-1}.

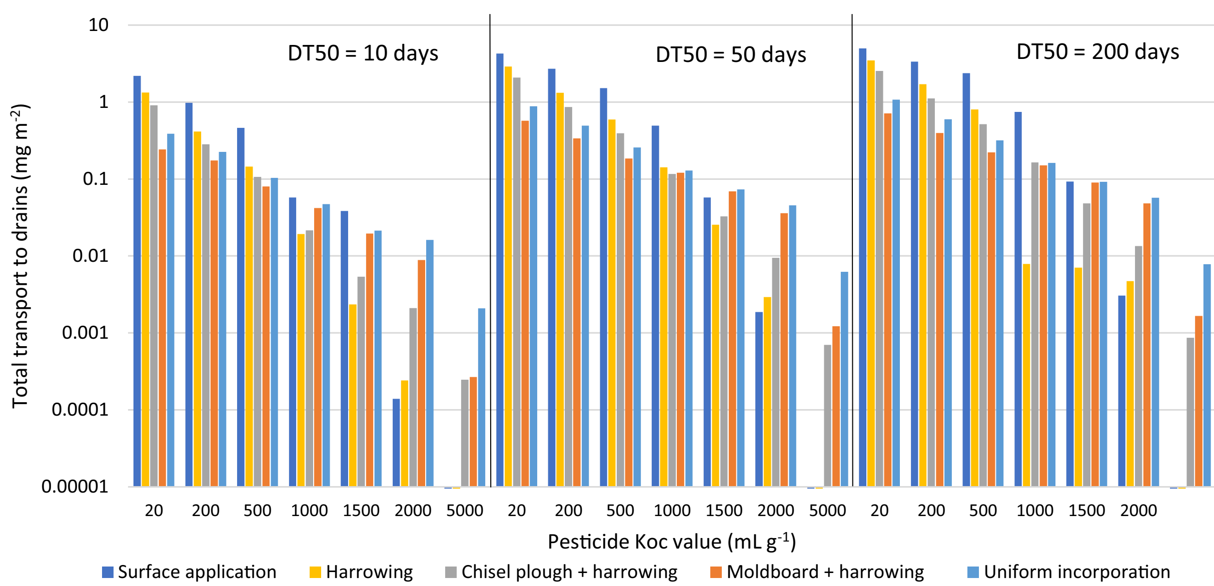

Figure 4. Seasonal loss of pesticide in drainflow (mg m^{-2}) simulated using MACRO 5.2 for different patterns of redistribution of pesticide residues in soil due to cultivation. Five cultivations patterns were simulated for pesticides with all combinations of Koc (20 to 5000 mL g^{-1}) and DT50 (10, 50 or 200 days). Results for pesticides with Koc = 5000 mL g^{-1} based on surface application and harrowing were < 0.00001 mg m^{-2}.

treatment yielding the least transport to drains varied with DT50 value and depending on whether maximum concentration (Fig. 3) or seasonal loss (Fig. 4) was considered.

Preferential flow is disproportionately important for the leaching of more strongly sorbed chemicals[38] where transport *via* matrix flow will be extremely limited. The fact that burying residues of more strongly sorbed chemicals (Koc ≥2000 mL g^{-1}) during cultivation increased subsequent transport to drains in our simulations appears contradictory. The observation may relate to the very sharp demarcation in soil properties in the D2 soil between the plough layer and the very slowly permeable subsoil.[32] Water and associated solute that reaches this horizon boundary will have a strong propensity for lateral movement and further channeling into structural macropores. Thus, it is likely that the model simulates a second zone with initiation of preferential flow at the base of the plough layer and that pesticide residues redistributed into this zone during cultivation will have increased availability for further vertical transport.

4 CONCLUSION

There is sufficient information in the literature to state that the primary redistributive effect of inversion (*e.g.* moldboard) ploughing will be to move the majority of any residues of pesticide present at or near the soil surface into the bottom two-thirds of the plough layer. In contrast, non-inversion (*e.g*. chisel) ploughing will have only a limited redistributive effect. Inversion ploughing remains an important cultivation practice for large areas of agricultural land because of benefits for weed control and consistency in generation of the seed bed. Recent research has presented a prototype model of the sort that will be necessary to extrapolate this redistributive effect of tillage from a limited set of experimental observations to a range of cultivation practices operating under different conditions in the field.[39] Further development and evaluation of mathematical models to describe the redistributive effect of soil cultivation should be a research priority, and it can be expected that this will then inform further research questions for empirical investigation in the field.

There is a likelihood that residues of some classes of pesticide that are applied relatively late in a cropping season will carry over in soil to the start of the next season. The instantaneous redistribution of soil residues that occurs during tillage will inevitably have an effect on subsequent fate and behavior of such pesticide residues. The analysis undertaken here demonstrates that subsequent leaching behavior will be modified to a large extent. Modelling suggests that the effect will depend on pesticide properties with more intense/deeper cultivation reducing the subsequent leaching of relatively mobile compounds, but increasing the leaching of relatively immobile compounds in heavy clay soils. This outcome from model simulations for a heavy clay with subsurface drains can be explained based on two zones of initiation for preferential flow - one zone at or near the soil surface, with the other at the base of the plough layer where the more permeable topsoil interfaces with the slowly permeable subsoil. Critically, the redistributive effect of different soil cultivation practices has been virtually ignored in the literature regarding the environmental fate of pesticides. There is an urgent need for field experiments to investigate the influence on pesticide leaching and to validate the model findings reported here. It will also be important to study a wider range of application timings and soil conditions, because the influence of a particular redistribution pattern on leaching will depend both on soil hydrology and on the main zones of interaction between pesticide and water moving through soil under any set of environmental conditions.

Whilst the findings reported here will need to be investigated in greater depth (for example, to assess influence of redistribution on fate predictions for other regulatory models such as PEARL), there could be important implications for environmental risk assessment procedures. Both maximum concentration and total loss of pesticide in drainflow when redistribution was included often changed by a factor of five to ten compared to the current risk assessment practice where redistribution is ignored. The standard regulatory modelling scenarios used for the authorization of pesticides in the EU were specifically created to represent conventionally tilled agriculture and to incorporate conservatism into their default parameterization. Given the significant impact of physical redistribution on modelling results and the role pesticide properties play in the scale of that impact, it is clearly an area of regulatory modelling which needs further consideration within the risk assessment when refinement of predicted environmental concentrations is considered appropriate.

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CONFLICT OF INTEREST DECLARATION

Mark Greener and David Patterson are employed by Syngenta Limited, the funder of this research.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

SUPPORTING INFORMATION

Supporting information may be found in the online version of this article.

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