



## Consequences of varied soil hydraulic and meteorological complexity on unsaturated zone time lag estimates



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### ABSTRACT

The true efficacy of a programme of agricultural mitigation measures within a catchment to improve water quality can be determined only after a certain hydrologic time lag period (subsequent to implementation) has elapsed. As the biophysical response to policy is not synchronous, accurate estimates of total time lag (unsaturated and saturated) become critical to manage the expectations of policy makers. The estimation of the vertical unsaturated zone component of time lag is vital as it indicates early trends (initial breakthrough), bulk (centre of mass) and total (Exit) travel times. Typically, estimation of time lag through the unsaturated zone is poor, due to the lack of site specific soil physical data, or by assuming saturated conditions. Numerical models (e.g. Hydrus 1D) enable estimates of time lag with varied levels of input data. The current study examines the consequences of varied soil hydraulic and meteorological complexity on unsaturated zone time lag estimates using simulated and actual soil profiles. Results indicated that: greater temporal resolution (from daily to hourly) of meteorological data was more critical as the saturated hydraulic conductivity of the soil decreased; high clay content soils failed to converge reflecting prevalence of lateral component as a contaminant pathway; elucidation of soil hydraulic properties was influenced by the complexity of soil physical data employed (textural menu, ROSETTA, full and partial soil water characteristic curves), which consequently affected time lag ranges; as the importance of the unsaturated zone increases with respect to total travel times the requirements for high complexity/resolution input data become greater. The methodology presented herein demonstrates that decisions made regarding input data and landscape position will have consequences for the estimated range of vertical travel times. Insufficiencies or inaccuracies regarding such input data can therefore mislead policy makers regarding the achievability of water quality targets.

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### 1. Introduction

The European Union Water Framework Directive (EU-WFD) (European Commission (EC), 2000) was enacted in December

2000. Its objective is to attain 'good' status for all surface and groundwater bodies by 2015, with the possibility to extend deadlines to the second reporting period in 2021 or beyond. The EU-WFD is enforced in member states through programmes of measures (POM) e.g. the Nitrates Directive in Ireland (EC, 1991), which aims to prevent water pollution by managing the use of fertiliser, manure and increasing nitrogen use efficiency (van Grinsven et al., 2012). In Ireland, the Agricultural Catchments

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Program (ACP) evaluates the environmental and economic effects of POM implemented under the Nitrates Directive (ACP, 2013). Despite prompt implementation of POMs throughout the EU in 2012, many catchments may not achieve good water quality status within the given timeframe, due to the time lag of nutrient transport from source to receptor via surface and subsurface hydrologic pathways. An appraisal of catchment time lag issues may offer a more realistic, scientifically-based timescale for expected water quality improvements in response to mitigation measures (Fenton et al., 2011; Jordan et al., 2005).

### 1.1. Time lag

Time lag ( $t_T$ ), also referred to as time delay, retardation factor, residence time, or memory effect (Bechmann et al., 2008; Cook et al., 2003; Fenton et al., 2011), is defined in this paper as the inherent hydrologic delay in response to mitigation measures. It is often conceptualised as consisting of both a vertical component through the unsaturated zone ( $t_u$ ) and a lateral component via the saturated zone ( $t_s$ ) (Sophocleous, 2012). It is acknowledged that the unsaturated zone also will inevitably contain a lateral component (Forrer et al., 1999), but for the purposes of this study  $t_u$  is assumed to represent vertical transport through the unsaturated zone alone. Furthermore the soil profiles used herein represent profiles in which this pathway prevails.

There is also evidence of time lag at larger national scales (e.g. Granlund et al., 2005 (Finland); Kronvang et al., 2008 (Denmark); van Grinsven et al., 2013 (EU)). Fenton et al. (2011), using saturated assumptions to various depths (maximum 10 m), demonstrated that  $t_T$  is likely to inhibit the capacity of many Irish catchments to achieve WFD targets within the designated reporting periods, and consequently, deadlines have been extended (Daly, 2011). However, site specific analyses incorporating variably saturated solute transport parameters would better account for the national diversity of soil and landscape conditions. Although it is often purported as a “generic excuse” (Scheure and Naus, 2010) to overcome more stringent policy measures, elucidation of time lag is fundamental in order to better predict the response of water bodies to a change in agricultural management practices (Meals et al., 2010; Mellander et al., 2012). In addition, catchments with the lowest time lags (high vulnerability) display a rapid response to POMs (e.g. free draining soils underlain by high permeability karst bedrock) (Huebsch et al., 2013) and offer an opportunity to test such POMs within specified reporting periods. Conversely, catchments with longer time lags (e.g. due to lower soil and aquifer permeability (Wang et al., 2012)), display slower responses limiting the potential to assess POM efficacy within the same reporting periods.

Numerous studies have highlighted the crucial role of the unsaturated zone within the hydrologic cycle, and the need for realistic quantification of  $t_u$  within hydrological models (Hooper, 2009; Torres et al., 1998; Vereecken et al., 2008). Sousa et al. (2013) described a methodology to assess the importance of  $t_u$  within the context of  $t_T$  (the sum of unsaturated and saturated time lags:  $t_T = t_u + t_s$ ) and advocated the use of measured rather than generic data collection to more accurately account for  $t_T$ . While it is typical within a catchment study for more investment and information to be readily available on  $t_s$  little

thought is often given to estimating  $t_u$ , despite the influence it exerts on solute transport timelines.

The focus of this paper is  $t_u$ , which is mainly controlled by soil/subsoil/bedrock type (Bejat et al., 2000; Helliwell, 2011), unsaturated thickness (Hillel, 2004), its variably saturated nature (Nielsen et al., 1986), interactions between the solute and the soil matrix (Leij and van Genuchten, 2011) and climatic factors (Diamond and Shanley, 2003; Stark and Richards, 2008). In addition, the spatial (Gumiere et al., 2013; Peck et al., 1977) and temporal variability (Mapa et al., 1986; Sousa et al., 2013) of weather and soil data and the proximity of a particular landscape position relative to ground and surface water receptors (Fenton et al., 2009, 2011; Jordan et al., 2005; Schulte et al., 2006; Sousa et al., 2013) are significant when determining the importance of  $t_u$ . Numerous studies (Baily et al., 2011; Fenton et al., 2011; Foussereau et al., 2001; Gladnyeva and Saifadeen, 2013; Huebsch et al., 2013; Premrov et al., 2014) have identified the critical influence exerted by meteorological patterns on  $t_u$ . Direct recharge (sometimes called effective drainage – Fenton et al. (2011)) to groundwater (and hence contaminant transport and  $t_u$ ) is implicitly linked with rainfall amount and soil/subsoil/bedrock permeability (Fitzsimons and Misteear, 2006).

### 1.2. Theoretical framework

#### 1.2.1. Unsaturated zone numerical modelling

Accounting for vertical transport presents a challenge due to the nonlinearity of unsaturated flow (Russo, 1991). A simple approach is to assume constant saturation (Fenton et al., 2011) (Eq. (1)). However, this is likely to underestimate  $t_u$ , as it fails to reflect the variably saturated nature of field conditions.

$$t_u = \frac{d}{ER/(n_e/100)} \quad (1)$$

where  $d$  (m) is depth of the soil profile,  $ER$  (m) is effective rainfall calculated after Schulte et al. (2005), and  $n_e$  is effective porosity (%). Fenton et al. (2011) demonstrated that for Ireland,  $t_T$  would exceed current EU-WFD reporting periods and, moreover, in some cases,  $t_u$  alone would be outside such periods. Sousa et al. (2013) represented the % of travel time spent in the unsaturated zone ( $t_r$ ) within the context of  $t_T$  (Eq. (2)).

$$t_r = \frac{t_u}{t_T} \quad (2)$$

In recent years, numerical models (free-licence and proprietary) capable of describing transport in the unsaturated zone have been developed (see reviews by Arheimer and Olsson, 2003; Jackson et al., 2006; Sousa et al., 2013). These models incorporate the Richards' equation for unsaturated flow and so better reflect field conditions than the saturated approach. Model selection must be based not only upon which best describes the process/problem in question, but also upon the data available and accuracy required (Konikow, 2011; Wagener et al., 2001). Models may simulate conservative solutes or include more complex solute transformation equations, such as in the UNSATCHEM module incorporated in the Hydrus series (Šimůnek et al., 1996).

Utilising such numeric models with the correct assumptions and boundary conditions (Vereecken et al., 2008), in conjunction with generic or measured soil physical characteristics and weather data as inputs (Keim et al., 2012; Sousa et al., 2013) (Fig. 1), can be an alternative to field tracer studies. Indeed, the latter allow for assessing the true  $t_u$ , but frequently are too labour intensive and costly to be conducted across large areas or across a variety of hydrologic conditions. Konikow (2011) noted that in addition to the financial demands of tracer tests, they may also have limited predictive capacity compared to numerical simulations. While assessing solute transport via these models is not new (Amin et al., 2014; Molénat and Gascuel-Oudou, 2002; Pang et al., 2000 and many others), limited consideration has been given to the effects of input data complexity and resolution on model outputs.

### 1.2.2. Meteorological data inputs

Modelling unsaturated zone processes based on atmospheric conditions requires meteorological inputs (precipitation, temperature, humidity, wind and radiation) to be supplied (Šimůnek et al., 2013). These determine the driving factors behind solute movement i.e. pressure head ( $h$ ) (cm) and volumetric water content ( $\theta$ ) (%) (Shipitalo et al., 2000). Studies have suggested that smaller time steps/greater resolution will result in more realistic simulations of water contents and pressure heads, and consequently may better account for solute movement (Gladnyeva and Saifadeen, 2013; Keim et al., 2012; Konikow, 2011; Wang et al., 2009).

### 1.2.3. Soil physical data inputs

Elucidation of soil-specific physical data (e.g. bulk density ( $B_D$ ), texture, pore size distribution) in the field or in the laboratory, or any knowledge of such properties from the literature, enables the soil hydraulic properties (residual water

content ( $\theta_r$ ), saturated water content ( $\theta_s$ ), and empirical parameters ( $m$ ,  $n$  and  $\alpha$ ) and saturated hydraulic conductivity ( $k_s$ ) to be inferred from the soil water characteristic curve (SWCC) using a fitting equation (e.g. van Genuchten-Mualem (VGM) (1980), Brooks and Corey (1964), Kosugi (1996), or Durner (1994)). Options (ranked from low to high complexity) used to determine the hydraulic properties are as follows: pedotransfer functions (PTF) such as the integrated soil catalogue (Carsel and Parrish, 1988) or Rosetta (Schaap et al., 2001), computational processes such as integrated particle swarm optimisation (IPSO) (Yang and You, 2013), or actual SWCC construction (0 to  $-15$  bar). All methods barring those employing actual SWCC infer hydraulic properties from known physical characteristics using fitting equations trained on extensive soil databases (Vereecken et al., 2010). The hydraulic parameters obtained through these various methods are used as inputs to numerical models.

Konikow (2011) suggested that increasing the complexity of a numerical model can improve the accuracy of its outputs (e.g. solute transport and hence  $t_u$ ), but at a cost of lowered ease of understanding and greater data demand. Similarly, increasing the complexity of data inputs to a model, such as by moving from pedotransfer functions to measured data, can likewise improve the performance of that model. Wösten et al. (1995) suggested that more complex soil data be employed only when the differences in estimates of soil behaviour were significant as a consequence. Mohamed and Ali (2006) found that using more detailed input data in PTFs increased their reliability. Several studies have noted failures of PTFs to wholly characterise the hydraulic behaviour of field soils (Khodaverdiloo et al., 2011; Schaap and Leij, 1998). According to such studies, moving from PTFs to actual measurements of the SWCC is therefore likely to improve estimates of soil hydraulic parameters, and hence produce more satisfactory simulations of in situ water and solute movement using numerical models.

### 1.3. Hypotheses and objectives

This paper examines the range of estimated  $t_u$  when a certain meteorological dataset at a certain temporal resolution is combined with various levels of input data (generic to soil profile and horizon-specific) derived through fitting of the VGM equation. A numerical model simulating a tracer injection through the soil profile can then be used to estimate a breakthrough curve (divided here into initial breakthrough (IBT), peak concentration (Peak), centre of mass (COM) and total exit of the solute (Exit)) at the base of a soil profile. The combination of these presents a comprehensive description of time lag. IBT can indicate when trend analysis (which is mandatory for 2021 reporting), should be initiated as it represents the initial contamination of the receptor after implementation of the POM. The COM equates most closely to saturated (Fenton et al., 2011) condition equivalents and indicates the period in which the greatest impact of the POM on the receptor will be observed. Exit is also important, as it represents the maximum residence time of the solute in the profile, subsequent to which a POM can be considered to have taken full effect.

Such information is essential to robustly estimate  $t_T$  and is vital to manage the expectations of policymakers and stakeholders throughout the  $t_u$  period by determining when POMs will begin to affect a receptor and when water quality targets

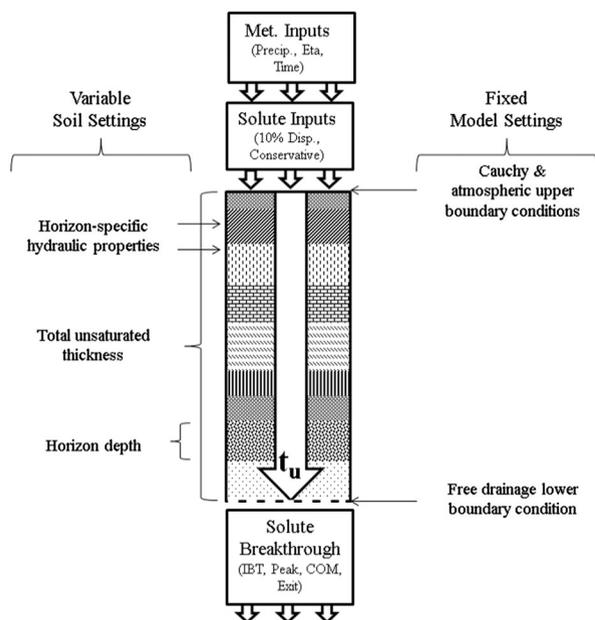


Fig. 1. Conceptual unsaturated numerical model diagram indicating input parameters, boundary conditions, horizon characteristics and model outputs.

may be attained (Tedd et al., 2014). Hydrus 1D (henceforth referred to as 'Hydrus'), a popular free-licence model for simulating the unsaturated zone, was selected to estimate  $t_u$ . Hydrus is a one-dimensional model with the capacity to be upgraded to more complex 2- and 3-dimensional simulations where sufficient data are available, and which can be coupled with a groundwater model (e.g. MODFLOW) to enable  $t_r$  estimation. As indicated by Sousa et al. (2013), the importance of the unsaturated zone component in the overall  $t_r$  estimation depends on many factors such as  $t_s$ , landscape position, and proximity to a surface receptor or groundwater abstraction point.

The first hypothesis of this paper is that modelled  $t_u$  in freely drained soils are less sensitive to decreases in the temporal resolution of weather data than in more poorly drained soils. The sensitivity of various soil textures to changes in temporal resolution will be examined, and recommendations will be made regarding the most appropriate time-step to be employed in Hydrus for the purpose of estimating time lag. The second hypothesis is as follows: increasing the level of complexity (generic to site-specific) employed to determine the soil hydraulic parameters using the VGM equation will add a higher degree of specificity to the soil hydraulic parameters and consequently improve  $t_u$  estimates. The final hypothesis is as follows:  $t_r$  will differ depending on landscape position, and this has consequences for the complexity of input data required. Therefore, the objectives were (a) to assess the sensitivity of various textural classes to changes in temporal resolution and make recommendations regarding the most appropriate time-step to be employed in Hydrus for the purpose of estimating  $t_u$ , (b) to assess the sensitivity of Hydrus to the complexity of soil input data and draw comparisons between the various complexity levels and (c) to use the Sousa et al. (2013) equation to assess the importance of data complexity in the unsaturated zone relative to various groundwater travel time scenarios; with  $t_r$  indicating the relative importance of  $t_u$  within the context of  $t_r$ .

## 2. Materials and methods

### 2.1. Model simulations

Hydrus 1D V4.16 (Šimůnek et al., 2013) was used for all model simulations to estimate vertical travel times of a conservative solute through homogenous and heterogeneous real-life soil profiles. Common to all simulations are the following: longitudinal dispersivity was set as the Hydrus default of 1/10th of the profile depth (Fetter, 2008; Šimůnek et al., 2013). Atmospheric boundary conditions with surface runoff and free drainage were imposed as the upper and lower boundary conditions, respectively (Jacques et al., 2008). A third-type/Cauchy solute upper boundary condition was imposed (Konikow, 2011; Šimůnek et al., 2013). A single-porosity, non-hysteretic VGM model was applied (van Genuchten et al., 1991). The threshold concentration at which IBT and Exit were considered to have been achieved was  $0.01 \text{ mmol cm}^{-1}$ . Centre of mass (COM) was calculated according to Payne et al. (2008). Meteorological data (hourly) from a synoptic station (Moorepark, Co. Cork;  $52^\circ 09' 50 \text{ N}$ ,  $08^\circ 15' 50 \text{ W}$ ) was obtained and the Penman–Monteith equation (Monteith, 1981; Monteith and Unsworth, 1990; Smith et al., 1991) was used to calculate evapotranspiration (Eta) based on measured precipitation, solar

radiation, humidity and windspeed, and assuming an albedo of 0.23 (grassland). This station was selected on account of its long-term, complete dataset, and its proximity and comparable weather patterns (Keane and Sheridan, 2004) to the sites in question. To initiate solute movement through the profile, 10 mm of precipitation was applied on Day 1, with a solute concentration of  $10 \text{ mmol cm}^{-1}$ . Fig. 1 provides a conceptual model for the Hydrus simulations. In Fig. 1 the variable soil input parameters are indicated on the right-hand side and the model settings applied across all simulations are indicated on the left-hand side. Model inputs (meteorological and solute) and outputs at the base of the soil profile (IBT, Peak, COM and Exit) are also depicted.

For hypothesis 1, hourly versus daily meteorological data time-steps (converted using SAS V9.1 (SAS, 2003)) from 2004 (a wet year, 1038 mm rainfall) and 2010 (a dry year, 763 mm rainfall) (mean annual Irish rainfall ranges from 750 mm to  $>1200 \text{ mm}$  (Keane and Sheridan, 2004)) were used in conjunction with homogeneous soil profiles, each of 0.5 m depth and each representing 12 textural classes (textural menu) and  $k_s$  ( $\text{cm h}^{-1}$ ) (Fig. 2). Such values were used as drainage class proxies, with lower permeability soils assumed to be more poorly drained than higher permeability soils (Gebhardt et al., 2009). Bulk density ( $B_D$ ) values for these textural classes were selected from the USDA soil quality test kit guide (USDA, 1999).

For hypothesis 2, transport through the unsaturated zone was simulated for 12 soil profiles surveyed as part of the Irish National Soil Survey (NSS) in the 1980s. The full dataset has been published by Diamond and Sills (2011). Table 1 presents abbreviated descriptions of these profiles. No field tracer experiments were conducted at these sites. However, the results of the present Hydrus simulations were compared with published values from a variety of lysimeter studies under similar meteorological conditions (e.g. Hooker, 2005; Kramers, 2009; Kramers et al., 2012; Richards et al., 2005; Ryan et al., 2001 – data presented in discussion herein, Selbie, 2013). The temporal resolution (2004–2008) of meteorological data was determined from the results of hypothesis 1. Simulations were conducted for each of the 12 NSS soil profiles using varying levels of soil physical characteristic data complexity to obtain the hydraulic parameters (Fig. 2). These were obtained via a range of simple to complex methods: textural class  $>$  ROSETTA  $>$  low pressure SWCC  $>$  full SWCC. The textural class parameters were selected from the Hydrus textural menu (Cassel and Parrish, 1988). ROSETTA was used to infer parameters based on sand, silt and clay percentages, and  $B_D$  (Diamond and Sills, 2011). The SWCC was fitted in RETC using the VGM equation, based on either the full curve (Diamond and Sills, 2011), or excluding the  $-15 \text{ bar}$  pressure step (low pressure).

### 2.2. Landscape position

For hypothesis 3,  $t_r$  was calculated according to Eq. (2) (Sousa et al., 2013). Exit was used to represent  $t_u$  for the purposes of estimating  $t_r$ ; next, each of the nine soil profiles were placed along a conceptualised catena (Anon, 2013) using their indicative soil groups from the NSS (Diamond and Sills, 2011). The transect ranges in soil group from podzol (typically higher up in the catena) to surface water and groundwater gleys (near a surface water receptor) (Anon, 2013). Saturated  $t_s$  values of 10, 5 and 0.5 years were used.

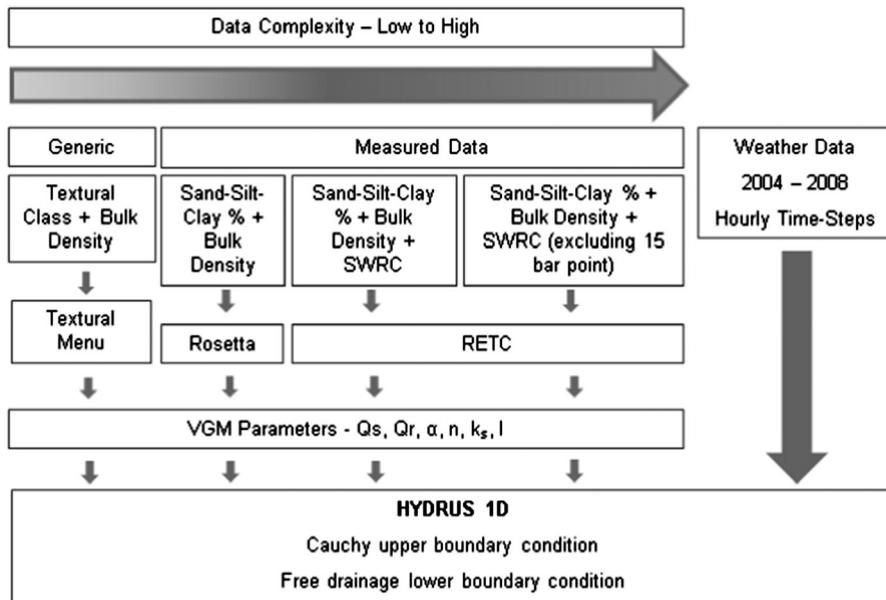


Fig. 2. Low to high complexity soil characteristic data employed in Hydrus 1D.

### 3. Results

#### 3.1. Meteorological data resolution

Table 2 presents tracer breakthrough times (IBT, Peak, COM and Exit) for hourly versus daily meteorological inputs (wet and dry year equivalents), combined with hydraulic property characteristics, for the 12 homogenous soil textural classes in the Hydrus textural menu. Hydrus simulations were successful from sand to loam ( $29.70$  to  $1.04$   $\text{cm h}^{-1}$ ), with variable success for heavier textured soils (silt loam ( $0.45$   $\text{cm h}^{-1}$ ) to clay ( $0.20$   $\text{cm h}^{-1}$ )). Sandy clay ( $0.12$   $\text{cm h}^{-1}$ ) to silty clay ( $0.02$   $\text{cm h}^{-1}$ ) consistently failed to converge. As  $k_s$  decreased, the model was less likely to converge, leading to failure  $<0.20$   $\text{cm h}^{-1}$  using a daily time-step and at  $<0.45$   $\text{cm h}^{-1}$  using an hourly time-step.

From sand to loam (better drained) regarding Exit: the temporal resolution of simulations (hourly and daily) produced

similar results for both wet and dry year equivalents, with IBT  $<0.04$  years. Irrespective of the soil textural range or wet/dry year simulation, the difference in IBT between hourly and daily simulations never exceeded  $0.01$  years. As expected, wet year IBT was quicker than the dry equivalent. Regarding Peak within the range of converging soil textures: differences between hourly and daily simulations ranged from  $0$  to  $0.07$  years. Average difference in Peak between hourly and daily simulations was  $0.02$  and  $0.01$  years for the wet and dry simulations, respectively. With the exception of the sand textural class (most freely drained), the differences between temporal simulations were greater for the wet year than for the dry year. For the soil textures which converged, greater differences between temporal resolutions were observed for COM,  $0.02$ – $0.28$  years. The difference in COM between the temporal resolutions for both wet and dry years was as follows: sand ( $0.02$  years for both wet and dry), loamy sand ( $0.03$  wet and  $0.06$  dry), sandy loam ( $0.06$  wet and  $0.13$  dry), sandy clay loam

Table 1

Summary of NSS (Waterford) soils.

Profile no.	Profile name	Soil great group (ISIS)	World Reference Base Classification	No. of layers	Depth m	$k_s$ range $\text{cm h}^{-1}$	Altitude m asl <sup>b</sup>	Saturated $t_u$ <sup>a</sup> Years
Non-converging	Lickey	Humic surface water gley	Haplic gleysol	6	1.00	0.15–7.90	145	0.35
Non-converging	Dungarvan	Typical luvisol	Haplic luvisol	9	1.60	0.11–1.02	30	0.39
Non-converging	Clashmore	Typical brown earth	Haplic phaeozem	8	0.90	0.13–0.92	80	0.29
9	Tramore	Typical surface water gley	Stagnic cambisol	5	1.20	0.22–0.45	55	0.88
8	Suir	Typical drained alluvial soil	Fluvisol cambisol	7	0.95	1.08–3.81	20	0.55
7	Slievecoiltea	Humic brown podzolics	Leptic cambisol	2	0.20	1.75–3.67	160	0.17
6	Portlaw	Humic podzol	Albic folic podzol	4	1.50	0.23–3.46	65	1.12
5	Newport	Typical surface water gley	Gleyic phaeozem	6	1.00	0.28–6.62	100	0.60
4	Kill 2	Typical brown earth	Haplic lixisol	7	1.00	0.20–2.27	65	0.75
3	Kill	Typical brown earth	Haplic lixisol	3	0.40	0.86–3.40	90	0.34
2	Callaghane	Typical brown podzolics	Haplic phaezoem	2	0.20	4.01–5.46	20	0.16
1	Ballymacart	Humic groundwater gleys	Haplic gleysol	9	1.25	0.40–8.13	90	0.77

<sup>a</sup> Fenton et al. (2011).

<sup>b</sup> Metres above sea level.

**Table 2**  
Daily vs. hourly estimates of IBT, Peak, COM and Exit for the 12 textural classes during a wet and a dry year respectively.

Textural class	$k_s$ cm h <sup>-1</sup>	IBT				Peak				COM				Exit			
		Wet year (2004)		Dry year (2010)		Wet year (2004)		Dry year (2010)		Wet year (2004)		Dry year (2010)		Wet year (2004)		Dry year (2010)	
		Daily	Hourly														
Sand	29.70	0.02	0.02	0.03	0.03	0.03	0.03	0.04	0.03	0.05	0.03	0.07	0.05	0.19	0.09	0.39	0.23
Loamy sand	14.59	0.02	0.02	0.03	0.03	0.04	0.03	0.04	0.04	0.07	0.04	0.12	0.06	0.24	0.18	0.53	0.25
Sandy loam	4.42	0.03	0.02	0.03	0.03	0.07	0.05	0.05	0.05	0.12	0.06	0.24	0.11	0.62	0.23	0.83	0.44
Sandy clay loam	1.31	0.03	0.02	0.03	0.03	0.10	0.03	0.09	0.07	0.24	0.09	0.37	0.17	0.81	0.31	No Exit (>1)	0.53
Loam	1.04	0.03	0.03	0.04	0.03	0.10	0.07	0.10	0.08	0.26	0.10	0.41	0.18	0.81	0.39	No Exit (>1)	0.55
Silt loam	0.45	0.04	a	0.04	0.03	0.13	a	0.09	0.08	0.38	a	0.50	0.22	1.00	a	No Exit (>1)	0.66
Clay loam	0.26	0.03	a	0.03	a	0.12	a	0.35	a	0.37	a	0.49	a	0.98	a	No Exit (>1)	a
Silt	0.25	0.04	a	0.04	a	0.15	a	0.41	a	0.39	a	0.52	a	1.00	a	No Exit (>1)	a
Clay	0.20	a	a	0.03	a	a	a	0.25	a	a	a	0.49	a	a	a	No Exit (>1)	a
Sandy clay	0.12	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
Silty clay loam	0.07	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
Silty clay	0.02	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a

<sup>a</sup> Failed to converge.

(0.15 wet and 0.20 dry), and loam (0.16 wet and 0.23 dry). The difference in COM increases as  $k_s$  decreases and is typically greater for dry years. Regarding Exit: the differences between temporal simulations ranged from 0.10 to 0.42 years for the wet simulation, and from 0.16 to 0.47 years for the dry simulation. The difference in Exit between the temporal resolutions for both wet and dry years was as follows: sand (0.10 years wet and 0.16 dry), loamy sand (0.06 wet and 0.28 dry), sandy loam (0.39 wet and 0.39 dry), sandy clay loam (0.50 wet and >0.47 dry (full Exit not achieved)), and loam (0.42 wet and >0.45 dry (full Exit not achieved)).

### 3.2. Soil hydraulic properties

For hypothesis 2 tables regarding the soil physical and hydraulic properties of all 12 NSS profiles are available as Supplementary data. As a complete example, Tables 3 and 4 show the soil physical and hydraulic properties, respectively, for Profile No. 1 (Ballymacart). As the textural menu and ROSETTA options do not indicate the actual SWCC of the soil, but rather infer hydraulic properties using pedotransfer functions, no  $r^2$  values are available to indicate how well the resulting VGM parameters describe the hydraulic properties of the specific soil in question. For both the full and low-pressure SWCCs,  $r^2$  values were typically >0.9, suggesting a very good fit of the curve for both datasets. For each individual horizon, the  $r^2$  for the full SWCC was not consistently greater than that of the low-pressure SWCC. Differences were observed in all hydraulic parameters derived using the textural menu and those obtained by fitting the SWCC. The textural menu assigned values according to textural class. Residual water content and  $k_s$ , determined using the textural menu, typically diverged from values elucidated from the SWCC. In the case of Profile No. 1,  $k_s$  was overestimated by 0.14 to 7.09 cm h<sup>-1</sup>, except for the EG horizons, in which it was underestimated by 2.75 to 3.54 cm h<sup>-1</sup>, while  $\theta_r$  was consistently overestimated. ROSETTA and both SWCC options showed good  $\theta_r$  agreement, but ROSETTA and the low-pressure SWCC diverged with respect to  $\theta_s$  relative to the full SWCC. The  $\alpha$  fitting parameter was considerably greater for the low-pressure than for the full SWCC. Changes to the fitting parameters allowed RETC to facilitate the fewer data points in the low-pressure SWCC relative to the full SWCC.

### 3.3. Solute breakthrough

For hypothesis 2, Fig. 3 shows the standard deviation (SD) in IBT, Peak, COM and Exit for each of the nine converging NSS profiles, according to the level of data complexity. The overall trend was that SD increased from IBT to Exit. Exceptions to this were in Peak for Profile Nos. 4, 5 and (marginally) 8. Standard deviation in IBT for each profile depending on input data complexity was typically small; ranging between 0.005 and 0.1 years. Profile No. 1 (Fig. 4A) showed the greatest difference in IBT depending on data complexity, with low complexity data overestimating the rate of IBT relative to the SWCC estimates (SD 0.1 years). Profiles No. 1 and No. 6 showed the greatest SD as regards solute Exit.

Fig. 4A–D shows IBT (A), Peak (B), COM (C) and Exit (D) for the nine converging NSS profiles. The bars indicate  $t_u$  in years determined according to the various data complexity levels.

**Table 3**  
Physical properties of Profile No. 1 (Ballymacart).

Horizon	Textural class	Depth cm	Sand %	Silt %	Clay %	$B_D$ g cm <sup>-3</sup>	$P_D$ g cm <sup>-3</sup>	$n_e$ %	Retained water % volume					
									0 bar	-0.002 bar	-0.059 bar	-0.137 bar	-1 bar	-15 bar
A1	Loam	0–10	47	47	6	1.00	2.26	34	59.5	52.8	47.7	45.4	40.1	21.3
A2	Loam	10–20	46	46	8	1.08	2.17	31	60.0	56.5	52.4	50.1	45.5	18.9
A3.1	Loam	20–30	47	47	6	1.22	2.25	26	50.7	48.7	46.1	45.1	40.6	19.4
A3.2	Loam	30–40	47	47	6	1.23	2.25	27	49.9	47.8	45.8	44.8	40.5	18.8
Eg1	Sandy loam	40–50	67	23	10	1.69	2.56	23	34.2	32.4	30.5	29.5	25.0	11.1
Eg2	Sandy loam	50–60	67	23	10	1.53	2.56	26	39.8	36.5	33.7	32.4	28.3	14.4
Bg1	Loam (silty)	60–80	59	32	9	1.51	2.65	33	43.3	37.5	34.1	32.6	25.3	10.3
Bg2	Loam (silty)	80–100	59	32	9	1.63	2.65	29	38.9	35.4	33.0	31.4	27.1	9.5
Cg1	Clay loam	100–125	45	32	23	1.50	2.64	17	49.1	43.6	41.7	40.8	37.6	25.8

Three of the 12 NSS profiles simulated failed to converge for some or all of the input complexity levels and so have been excluded from the results. Specifically regarding IBT, the differences between each complexity level were typically minor (0.01–0.05 years) with the exception of Profile No. 1 (0.22 years). Peak concentration and COM were influenced by data complexity for most profiles (Fig. 4B and C). Differences in COM between the low pressure and full SWCC simulations were typically minor (SD 0.12 years), except for Profiles No. 1 (0.32 years) and No. 6 (0.24 years) (Fig. 3). There is a trend for underestimation of COM as data complexity is decreased relative to the SWCC simulations (Fig. 4C). Greater differences in COM are observed for the deeper and more layered profiles (e.g. Profile No. 1) than for the shallow, more homogeneous profiles (e.g. Profile No. 2 – SD of 0.03 years) (Fig. 3). The greatest SD amongst the four data complexity levels were found regarding solute Exit (i.e. 0.32 years, Figs. 3/4D). As with COM, there was a trend for underestimation of solute Exit when low complexity data were employed, compared to using SWCC data. Differences between full and low pressure SWCCs were greatest for Profile No. 1 (0.66 years), but relatively minor for all other profiles (<0.19 years, Fig. 4D). Estimates of Exit based on low complexity data underestimated those based on the full SWCC by between 0.28 and 0.97 years (Fig. 4D). Saturated equivalent  $t_u$  (Table 1) underestimated those based on the full

SWCC (Fig. 4D) by 0.34 to 1.71 years. Underestimation was typically greater for deeper profiles (e.g. Profile Nos. 1, 4 and 6).

### 3.4. Landscape position

Based on the Sousa et al. (2013) equation, the  $t_r$  depending on data complexity using  $t_s$  of 0.5, 5 or 10 years is shown in Table 5. Shorter  $t_s$  led to greater  $t_r$  for all profiles. Increasing the input data complexity led to increases in calculated  $t_r$ . Using low complexity data, as opposed to the full SWCC, led to underestimation of  $t_r$  by up to 28%, 10% and 7% for  $t_s$  values of 0.5, 5 and 10 years, respectively. Only the shallow profiles (Profile Nos. 2, 3 and 7) typically displayed  $t_r$  values <10%. Differences in  $t_r$ , depending on whether the full or low pressure SWCC was used, were typically minor (<6%). Fig. 5A shows the nine NSS profiles placed relative to a surface receptor on a conceptualised catena. The landscape position of Irish soil types is shown in Fig. 5B, with those NSS profiles simulated herein, highlighted. The  $t_r$  values shown represent the potential range of  $t_r$  calculated according to soil characteristic data complexity. As distance from the surface water receptor and  $t_s$  increased, there was a general trend towards decreasing  $t_r$ , despite increasing  $t_u$  (e.g. Profile Nos. 1 and 6 versus 2). However, even at the maximum simulated distance from the receptor ( $t_s$  10 years),  $t_r$  consistently exceeded 10%.

**Table 4**

Hydraulic properties of Profile No. 1 (Ballymacart) determined from the textural menu, ROSETTA and by fitting of the full and low pressure SWCC.

Horizon	$\theta_r$	$\theta_s$	$\alpha$	n	$k_s$ (cm h <sup>-1</sup> )	R <sup>2</sup>	$\theta_r$	$\theta_s$	$\alpha$	n	$k_s$ (cm h <sup>-1</sup> )	R <sup>2</sup>
Textural menu						ROSETTA						
A1	0.078	0.430	0.036	1.56	1.04	n/a	0.043	0.452	0.007	1.58	8.13	n/a
A2	0.078	0.430	0.036	1.56	1.04	n/a	0.045	0.436	0.007	1.58	5.21	n/a
A3.1	0.078	0.430	0.036	1.56	1.04	n/a	0.038	0.396	0.009	1.54	3.35	n/a
A3.2	0.078	0.430	0.036	1.56	1.04	n/a	0.038	0.394	0.009	1.54	3.22	n/a
Eg1	0.065	0.410	0.075	1.89	4.42	n/a	0.038	0.333	0.043	1.36	0.88	n/a
Eg2	0.065	0.410	0.075	1.89	4.42	n/a	0.042	0.374	0.033	1.45	1.67	n/a
Bg1	0.067	0.450	0.020	1.41	0.45	n/a	0.038	0.364	0.026	1.42	1.40	n/a
Bg2	0.067	0.450	0.020	1.41	0.45	n/a	0.035	0.337	0.033	1.36	0.91	n/a
Cg1	0.095	0.410	0.019	1.31	0.26	n/a	0.064	0.393	0.014	1.43	0.40	n/a
Full SWCC						Low pressure data – no – 15 bar point						
A1	0.043	0.560	0.023	1.14	8.13	0.93	0.043	0.595	5.621	1.04	8.13	0.98
A2	0.045	0.554	0.001	1.36	5.21	0.96	0.045	0.598	1.070	1.04	5.21	0.98
A3.1	0.038	0.481	0.001	1.32	3.35	0.98	0.038	0.499	0.066	1.05	3.35	0.97
A3.2	0.038	0.474	0.001	1.34	3.22	0.98	0.038	0.490	0.046	1.05	3.22	0.96
Eg1	0.038	0.322	0.002	1.31	0.88	0.98	0.038	0.334	0.032	1.08	0.88	0.97
Eg2	0.042	0.372	0.006	1.45	1.67	0.95	0.042	0.397	2.024	1.04	1.67	0.96
Bg1	0.038	0.399	0.012	1.22	1.40	0.95	0.038	0.431	2.842	1.10	1.40	0.91
Bg2	0.035	0.352	0.002	1.39	0.91	0.95	0.035	0.387	1.982	1.04	0.91	0.95
Cg1	0.064	0.460	0.016	1.43	0.40	0.91	0.064	0.491	66.423	1.02	0.40	0.97

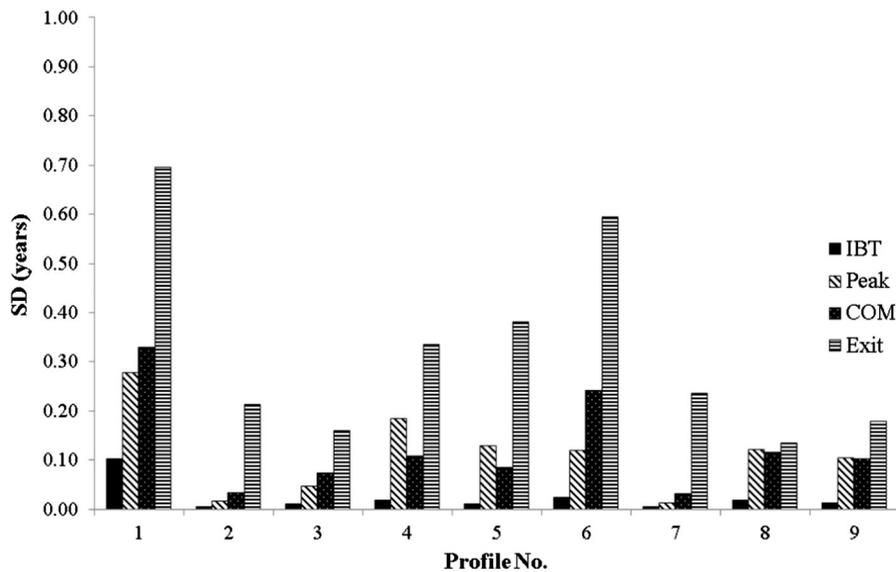


Fig. 3. Standard deviation (SD) in IBT, Peak, COM and Exit for each of the 9 NSS profiles, depending on data complexity.

## 4. Discussion

### 4.1. Meteorological data resolution

The failure of the model to converge when simulating low  $k_s$  soils indicates that hypothesis 1 can only be assessed in soils with less clay and silt contents i.e., more freely drained soils with a more dominant vertical component, and furthermore, suggests that the model may not be ideally suited for the assessment of  $t_u$  in high clay content soils i.e. with imperfectly or poorly drained profiles. Such a limitation has been well documented in the literature (Chiu and Shackelford, 1998; Vereecken et al., 2010). However, it is reasonable to assume that in such 'heavy' soils (which represent 32% of Irish agricultural soils; Humphreys et al., 2008), or those soils possessing a low permeability layer at shallow depth (e.g. due to natural or anthropogenic reasons), mixed contaminant nutrient losses to a surface waterbody are more likely to occur through overland flow rather than sub-surface pathways (Doody et al., 2006; Fleige and Horn, 2000; Ibrahim et al., 2013; Kurz et al., 2005a, 2005b). Within the range of converging textures (i.e.  $>0.20 \text{ cm h}^{-1}$ ) there is a greater need for higher temporal resolution of meteorological data, as the  $k_s$  of the soil profile (or of specific layers) decreases. This confirms hypothesis 1; that freely drained soils are less sensitive to the temporal resolution of meteorological data than poorly drained soils.

Critical for trend analysis is that temporal resolution is not vital when estimating IBT (differences  $<0.04$  years) (Table 2), which means that a daily time step can be utilised. However, as COM is of primary interest with respect to testing the efficacy of POMs, the hourly time-step is most appropriate (Fenton et al., 2011). Mertens et al. (2002) found that increasing temporal resolution of weather data improved estimates of runoff obtained using Hydrus 1D. Similarly, Gladnyeva and Saifadeen (2013) found that lower temporal resolution led to errors in estimates of the COM of transported solutes both for hysteretic

and non-hysteretic simulations. This is in agreement with the general hydrologic modelling recommendations of Konikow (2011). Furthermore, meteorology and rainfall intensity were shown to play a critical role in determining the rate and nature of solute movement and eventual recharge to groundwater and hence, should be accounted for in numerical models (e.g. Baily et al., 2011; Fenton et al., 2011; Gladnyeva and Saifadeen, 2013; Huebsch et al., 2013; Jahangir et al., 2013; Keim et al., 2012; Kramers et al., 2012; Misstear, 2000; Pot et al., 2005; Schulte et al., 2006; Torres et al., 1998). By increasing time-step, the user essentially averages precipitation over a greater duration, which poorly reflects the intensity of the event and consequently results in errors in model outputs.

Hydrus has the capacity to accept meteorological inputs in the form of 'time variable boundary conditions' (TVBCs), in various time units. However, the graphical user interface (GUI) in Hydrus is limited to 10,000 TVBCs. Consequently, when hourly inputs are supplied, the simulation is limited to 10,000 h (1.14 years). For many soil profiles, this is an insufficient length of time to wholly account for solute exit from the profile. Alternatives to overcome this limitation are as follows: (a) to manually input additional TVBCs outside of the GUI, (b) to use a lower time resolution such as a daily time-step, or (c) to use the end conditions from the initial simulation as initial conditions for a subsequent simulation. In addition to the daily and hourly temporal resolutions and results presented here, simulations were conducted using 2, 4, 6 and 12-h temporal discretisation (interim time-steps). However, the results of those simulations were not included as they became increasingly dissimilar to those obtained using daily or hourly time-steps as temporal resolution decreased, i.e. with the 2-h discretisation being most similar and the 12-h being most divergent. While it may be tempting to simply reduce the temporal resolution of weather data, the authors found that this practice led to substantial discrepancies in parameter estimation. It is likely that these errors result from discrepancies between the time-steps over

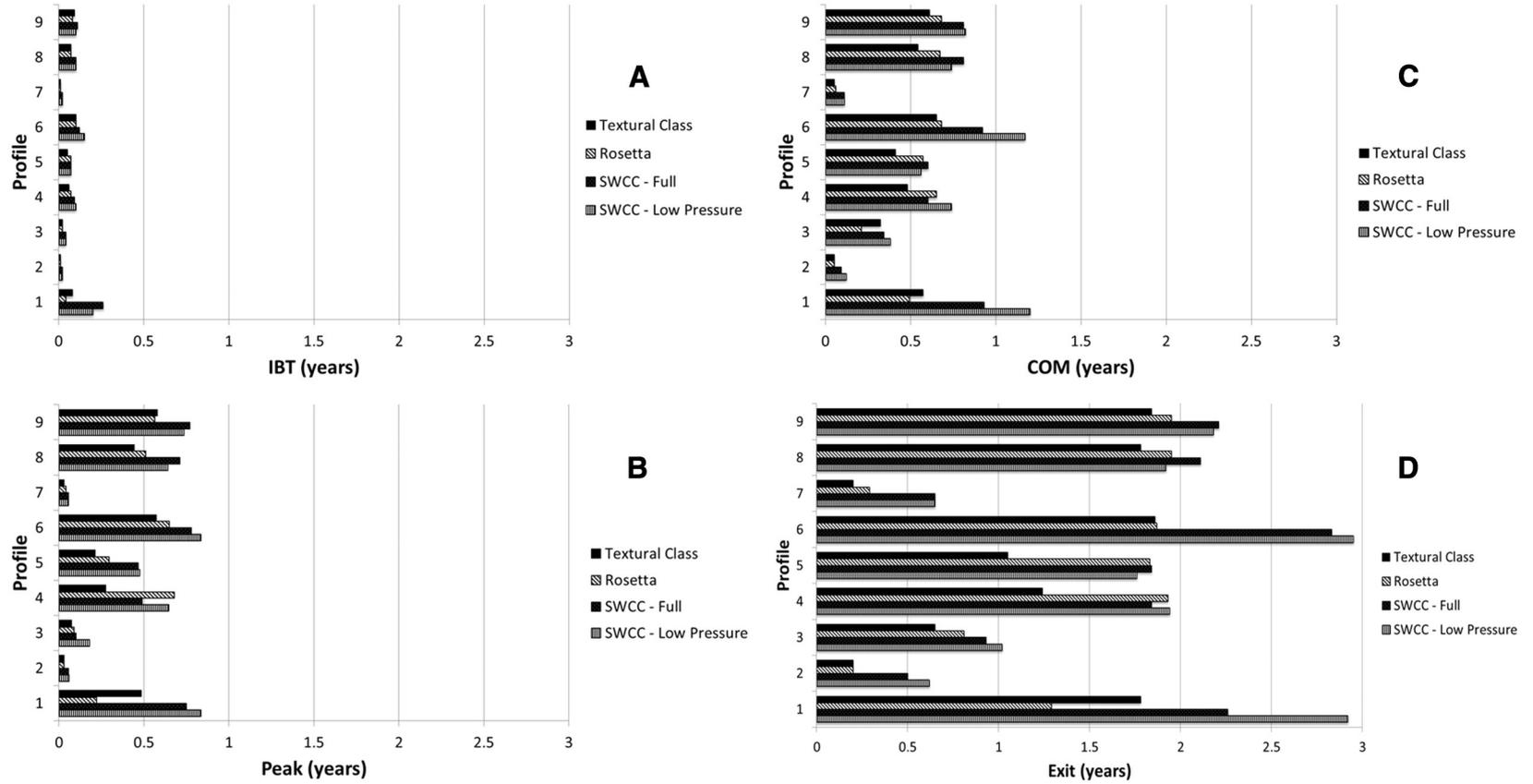


Fig. 4. Top to bottom: A) IBT, B) Peak, C) COM and D) Exit for the NSS profiles using simple to complex input data.

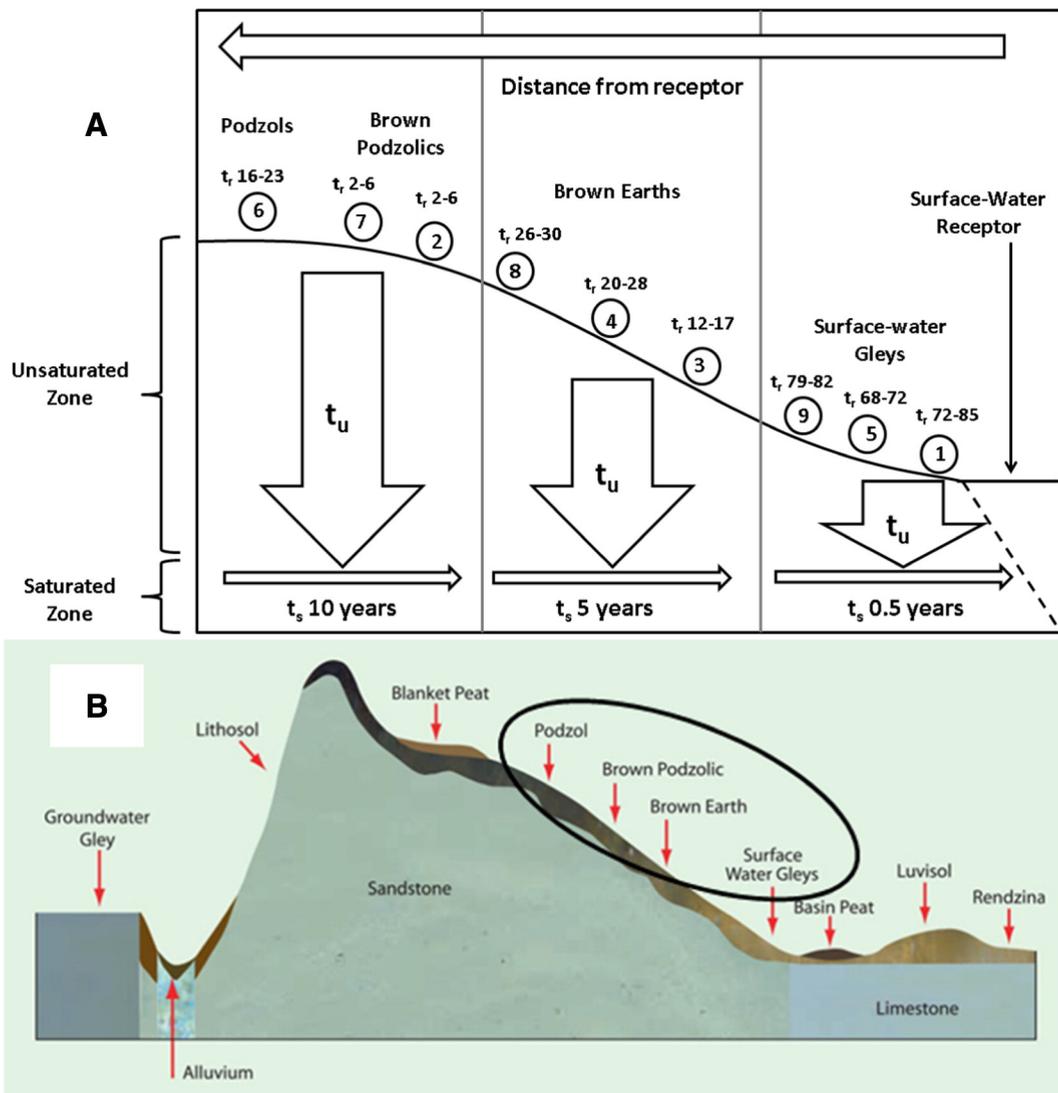
**Table 5**

Importance of  $t_u$  relative to total time lag ( $t_r$ ) in % ( $t_r$ ) across data complexity range, when the saturated time lag ( $t_s$ ) varies (0.5, 5 and 10 years).

Profile no.	$t_s$ (years)											
	0.5 (near receptor)				5 (mid slope)				10 (hillslope)			
	Textural menu	Rosetta	Low pressure	Full	Textural menu	Rosetta	Full	Low pressure	Textural menu	Rosetta	Low pressure	Full
9	79	80	81	82	27	28	31	30	16	16	18	18
8	78	80	79	81	26	28	30	28	15	16	16	17
7	29	37	57	57	4	5	12	12	2	3	6	6
6	79	79	86	85	27	27	36	37	16	16	23	22
5	68	79	78	79	17	27	27	26	10	15	15	16
4	71	79	80	79	20	28	27	28	11	16	16	16
3	57	62	67	65	12	14	16	17	6	7	9	9
2	29	29	55	50	4	4	9	11	2	2	6	5
1	78	72	85	82	26	21	31	37	15	11	23	18

which the boundary conditions are imposed (Šimůnek, 2014). For scenarios where solute breakthrough is likely to exceed 10,000 TVBCs, instead of attempting to overcome the limitations

of the GUI by decreasing the temporal resolution, input data is best supplied outside of the GUI. The failure of these interim time-steps to produce satisfactory results is, in reality, unlikely to



**Fig. 5.** A) Position of NSS Profile Nos. 1–9 relative to a surface receptor and  $t_r$  ranges. B) Position of various soil types relative to a surface receptor. Soils simulated in this paper (podzol to surface water gleys) are highlighted.

Adapted from Anon (2013).

be a significant problem to model users, as meteorological data are typically available in daily or hourly resolutions.

The difference in solute Exit and COM between daily and hourly simulations (Table 1) suggests that hourly data may better simulate solute movement. While the difference in COM between simulations increased with decreasing  $k_s$ , this was not the case with Exit. As COM represents the bulk of solute movement, this result confirmed the hypothesis that sensitivity to temporal resolution is greater in more poorly drained soils. The failure of Exit to conform to this pattern may be as a result of the physical retardation of solute movement through areas of restricted flow (Kartha and Srivastava, 2008; Kramers et al., 2012), as a result of low mobile water content (Konikow, 2011; Padilla et al., 1999) or decreased porosity. However, the solute concentrations observed during the tailing period are extremely low and unlikely to contribute significantly to groundwater contamination. This of course must be tested further by incorporating data in future time lag analyses on nitrate transformational processes or phosphorus adsorption/desorption dynamics. The initiation of this tailing effect corresponded with the driest period of the year, in which differences in  $h$  between the hourly and daily simulations were greatest (up to 124 cm). The failure of Profile Nos. 4, 5 and 8 to conform to the overall trend of increasing SD of COM relative to Peak (Fig. 3) is indicative of the limited extent of tailing present; with those profiles exhibiting greater tailing (e.g. Profile No. 1) also exhibiting a greater SD as regards COM relative to Peak.

Co-location of meteorological stations and collection of soil physical data are important, as the spatial variability of weather within/across catchments and indeed larger areas can be considerable (Mapa et al., 1986; Sweeney, 1985). In addition, potential errors in site-specific values resulting from unequal distribution of synoptic recording stations can be problematic. In Ireland, synoptic recording stations are both limited in number and unequally distributed across the country, thus limiting the spatial accuracy of weather recording. This difficulty may be offset by supplying precipitation data from the c. 750 rainfall recording stations, which are well distributed. The evapotranspiration parameters, which exhibit lower spatial variability, can be interpolated from Met Éireann's (the Irish meteorological service) 25 synoptic stations. A digital elevation model, such as that described by Goodale et al. (1998), may aid in this. However, in vulnerable catchments, site-specific meteorological data, coupled with actual soil data, will help to elucidate more reliable ranges of  $t_u$ .

#### 4.2. Soil hydraulic properties

Considerable differences were observed in the soil hydraulic properties determined via the textural menu, ROSETTA and the full and low-pressure SWCCs, respectively. Assuming that the full SWCC furnishes the most appropriate soil hydraulic properties to describe a specific soil, it is clear that using generic values, such as those obtained via the textural menu, can lead to significant errors, and may poorly reflect the properties and consequently processes of a specific soil. These values should at best be considered to give a rough indication of likely solute transport conditions, and may be adequate to estimate IBT (Table 4). From policy makers' point of view, IBT (or trend) is vital as it indicates the initial response of a receptor to a POM and hence informs scientists when their monitoring

network can begin to pick up the POM signal. As SD of this marker did not exceed 0.10 years for any of the profiles herein, it seems imminently practical to accept low complexity, textural data as the preferred input variable. However, such low complexity data appears to be wholly insufficient when bulk effect of POM can be observed by the monitoring network. This is important as POM efficacy can only be assessed by analysing data collected during the COM period. Therefore, the correct identification of COM requires selecting more complex options as described herein (Fig. 2).

The textural menu method also leads to a homogenising effect on the hydraulic properties of the various horizons within a single profile, and hence may not wholly reflect changes in water and solute movement patterns as influenced by particle size distribution or  $B_D$  within a single textural class, e.g. horizons A1 and A2 of Profile No. 1 (Table 4). The ROSETTA method was more satisfactory, bearing closer resemblance to the SWCC results. For example, horizon A1 of Profile No. 1 displays  $\theta_s$  values of 0.430, 0.452 and 0.560 according to the textural class, ROSETTA and SWCC methods respectively. Likewise,  $k_s$  values for that horizon were estimated as 1.04, 8.13 and 8.13  $\text{cm h}^{-1}$  respectively, depending on input data complexity. Hence, the ROSETTA method can be assumed to more closely reflect hydraulic properties than textural class-based estimates. However, this method still represents a simplified description of the soil and, as resulting  $\theta_s$  values diverged from those obtained using the SWCC, could lead to errors in water and solute transport calculation. Regarding the full and low-pressure SWCCs, reasonable similarity was observed between the two, and both presented high  $r^2$  values ( $>0.90$ ), suggesting a good fit of the SWCC using the VGM equation. By removing the  $-15$  bar pressure point, the VGM equation maintained a good fit, but compensated by increasing the  $\alpha$  parameter, e.g. from 0.001 to 1.070 in horizon A2 of Profile No. 1 (Table 4). In reality, measurement of the  $-15$  bar pressure step is arduous, slow and expensive. This step may be excluded when IBT, Peak and COM are of primary concern. This pressure step is only essential for estimation of total solute Exit (Fig. 4D).

#### 4.3. Solute breakthrough

##### 4.3.1. Validity of Hydrus simulations

The failure of three profiles to converge was related to the clay content and low  $k_s$  of their lower horizons. This corresponds to failures documented in Section 3.1. For these NSS soils, nutrient loss is unlikely to occur through the vertical pathway, with runoff, lateral transport and increased dispersion through the subsurface prevailing (Blanco-Canqui and Lal, 2008; Jarvis et al., 2007; Kramers et al., 2012; Kurz et al., 2005a, 2005b). Consequently, Hydrus 1D is not the optimum model for the simulation of solute transport in these soils.

It must be acknowledged that the values of  $t_u$  presented here, regardless of input data complexity employed, do not represent the exact duration of solute movement through the profile. A model is only 'a simplification of a very complex reality' (Konikow, 2011). Due to the complexity and dynamic nature of contributing factors, time lag estimates can, at best, provide ranges in which response can be anticipated (Meals et al., 2010). Furthermore, as the Richards equation upon which the Hydrus single-porosity model is based (Šimůnek et al., 2013) neglects the occurrence of preferential flow, resulting

estimates such not be assumed to preclude discrepancies in solute breakthrough, particularly as regards IBT, in structured soils. In such soils, more rapid solute movement may be observed as a consequence of preferential flow (Gerke, 2006; Kramers, 2009; Kramers et al., 2012), in which case the application of a dual-porosity or permeability model within Hydrus may be more appropriate.

While measured breakthrough curves are not available for the NSS profiles described here, numerous studies under similar soil and meteorological conditions have demonstrated that the results obtained from the Hydrus simulations are likely to be realistic and within the ranges observed during unsaturated tracer and lysimeter experiments (Ryan et al., 2001; Hooker, 2005; Richards et al., 2005; Kramers et al., 2012; Selbie, 2013). In particular, the lysimeter study by Kramers et al. (2012) was conducted using soils which are closely comparable to those detailed herein.

Table 6 shows results (Peak, COM and Exit) from Kramers et al. (2012) – presenting IBT and recovery using 1 m-deep lysimeter profiles ( $n = 4$ ). Lysimeters were exposed to an average yearly rainfall of 879 mm during that study. While direct comparison of the NSS profiles and those described by Kramers et al. (2012) cannot be drawn as they are essentially discrete sites, there are considerable physical resemblances between them, and both datasets originate from similar climatic and pedogenic environments. The Oak Park soil is roughly analogous to Profile Nos. 2 and 3. The Clonroche and Elton soils resemble Profile Nos. 5, 6 and 9. The poorly drained Rathangan soil is most similar to Profile Nos. 1 and 8. Kramers et al. (2012) found IBT of <0.08 years for all profiles, which compares favourably with the Hydrus NSS simulations (est. IBT typically <0.09 years, except in the case of Profile Nos. 1 and 7). Peak concentration in the NSS soils occurred on average between 0.30 and 0.50 years, which closely resembles peaks observed in the Oak Park and Clonroche soil in the lysimeter study. Peak occurrence for the Elton soil exceeded this for the spring application (0.85 years), but so too did the equivalent Profile Nos. 6 and 9 with peak occurrence ranging between 0.58–0.84 and 0.57–0.77 years, respectively (depending on data complexity). Comparing Exit and COM for the Oak Park and Clonroche soils with the results of the data complexity trial suggests that the low complexity data likely underestimates these parameters, and that the high complexity data may result in more realistic estimates. Total solute exit from the Clonroche soil was not achieved during the experimental timeframe of 1.14 years (Kramers et al., 2012); Exit from the equivalent NSS profiles likewise exceeded this duration regardless of data complexity. Due to the poor recovery of the  $\text{Br}^-$  tracer from the Elton and Rathangan soils, the COM and Exit values should not be considered to wholly reflect the total exit of solute from these profiles, which exceeded the experiment duration. Kramers et al. (2012) observed a decrease

in  $\text{Br}^-$  recovery as the drainage class of the soils decreased (Oak Park > Clonroche > Elton > Rathangan). There is a similarity between the failure to recover the tracer from this profile and the failure to converge of the three heavy NSS soils. This also reflects the slower Exit observed in the Hydrus simulations as clay content increased and  $k_s$  decreased. This gives further evidence to suggest that heavy clay soils are less at risk through the vertical as opposed to lateral pathways, and so their contribution to water contamination is likely to be insufficiently accounted for by one dimensional, vertical model. The results of the SWCC simulations more closely resembled the lysimeter results than those obtained using low complexity data, suggesting that measurements of the SWCC may result in more realistic simulations of actual soil profiles than are obtained via generic, pedotransfer functions. The low complexity data typically resulted in quicker Exit than was observed in comparable lysimeter studies.

#### 4.3.2. Comparison of simple to complex input data

Regarding the Hydrus simulations of the NSS profiles, a general trend was observed in which underestimation of Exit and COM increased as data complexity decreased relative to the full SWCC simulations (Figs. 3, 4C and D). Decreases in complexity resulted in underestimation of Exit by 0.28 to 0.97 years, and in COM by 0.02 to 0.36 years. These errors reflect the limited ability of low complexity data to describe the hydraulic behaviour of specific soils compared to measured values. Likewise, the general trend for increasing SD as regards COM and Exit relative to IBT and Peak suggests that detailed soils data are more critical where estimation of these markers is intended (Fig. 3). Consequently, high quality, measured soil data are required to make site-specific estimates of time lag. Unsaturated estimates exceeded saturated estimates (Fenton et al., 2011) from between 0.34 and 1.71 years. As these estimates performed more poorly in the deeper profiles (e.g. Profile Nos. 1, 4 and 6), it should be considered that where the soil layer is thicker, unsaturated conditions are likely to play a greater role in determining solute transport (Sousa et al., 2013). The unsaturated simulations, while still representing a simplified conceptualisation of water and solute movement, suggest that generic soil characteristics and saturated assumptions vastly underestimate time lag, and are likely to lead to unrealistic expectations regarding groundwater remediation timeframes.

The differences in Exit for the NSS profiles between data complexity levels were greatest for deeper soils displaying many horizons; e.g. Profile No. 1. Therefore, for very simple, shallow profiles high data complexity may be less critical. Likewise, where IBT of the solute is of primary interest, low complexity data may suffice. Sousa et al. (2013) noted that the importance of potential underestimation of  $t_u$  depends on 'the

**Table 6**  
Summary results of Kramers et al. (2012) lysimeter study.

Profile name	Description	World Reference Base Classification	Drainage class	IBT	Peak	COM	Exit	Tracer recovery
				Years				%
Oak Park	Sandy loam (0.45 m) over gravel	Haplic cambisol	Freely drained	0.08	0.37	0.38	0.99	86
Clonroche	Moderately structured loam	Haplic cambisol	Relatively well drained	0.05	0.56	0.61	>1.14	70
Elton	Structured loam/silt loam	Cutanic luvisol	Moderately well drained	0.04	0.84	0.67	1.07	54
Rathangan	Loam to clay loam	Luvic stagnosol	Poorly drained, some gleying	0.01	0.02	0.18	1.10	33

context of other uncertainties', and of the potential cost of more detailed analyses, such as measuring the SWCC.

Differences in Exit between full and low pressure SWCC data inputs were typically small – on average 0.08 years. Only one profile (Profile No. 1) exhibited a large difference in Exit depending on the presence or omission of the – 15 bar value from the SWCC (Fig. 4D). From a monitoring perspective, the signal is likely to be so low that it will be difficult to connect such concentrations with specific nutrient losses from the surface. This makes Exit interesting from a theoretical point of view, but in reality will not inform expectations of policy makers with respect to time lag and simply plays into the “generic excuse” category.

#### 4.4. Landscape position

It is clear from Table 5 and Fig. 5A, that even when  $t_s$  is large, the unsaturated zone is always important, and so must typically be accounted for when assessing  $t_r$ . The effect of data complexity on  $t_r$  demonstrates that where  $t_s$  is shorter, such as when the unsaturated zone is underlain by karst geology (Drew, 2008), the use of high complexity data is more critical. Conversely, where  $t_s$  is slow, there may be grounds for a decrease in data complexity. Only the profiles with the most rapid  $t_u$  in conjunction with large  $t_s$  exhibited small  $t_r$  values. This suggests that  $t_u$  is of critical importance for most profiles, and so high quality data are recommended.

Based on Fig. 5A, it is clear that  $t_r$  is influenced not only by the properties of the unsaturated zone, but also by landscape position. Hence, this factor should also be taken into account when surveying a site for the purpose of determining  $t_u$ , and this may inform the level of data complexity employed. For example, where a shallow profile is distant from the receptor, a decrease in data complexity, which would allow a judicious use of time and resources, may be beneficial. This is in accordance with Sousa et al. (2013), who suggested that there is no obvious threshold at which  $t_u$  becomes critical or negligible, but rather that the timescales involved, cost of additional data acquisition and importance of the receptor (from an abstraction or environmental point of view) should be considered. Consequently, decisions regarding the optimum level of soil data complexity can only be made on a case-by-case basis. The greater context of the profiles simulated herein is demonstrated in Fig. 5B, which identifies the likely position of these profiles relative not only to a surface water receptor, but also to other common soil types. The NSS profiles (highlighted) are representative of those Irish soil types most likely to contribute to water contamination through the vertical dimension.

The small differences in  $t_r$  between the full and low pressure SWCC (<6 years) (Table 5) suggests that in many instances, it may not be necessary to measure the entire curve. The – 15 bar pressure point is extremely time consuming and difficult to obtain using traditional methods such as pressure plates (Cresswell et al., 2008; Gee et al., 2002; Madsen et al., 1986). The difficulty in measuring this point has contributed in part to the popularity of pedotransfer functions (Fredlund and Xing, 1994; Saxton et al., 1986; Vereecken et al., 2010), but as is shown here, this comes with a loss of site-specific accuracy. Measuring the SWCC excluding this point may present the optimum method of determining  $t_u$ . This will be further investigated as part of the current study.

## 5. Conclusions

For determining the potential impact of activities in a sensitive catchment, policy makers need to consider the type of data required to model the movement of water through the soils. Where initial (trend analysis) or peak breakthrough of a contaminant is the primary concern, use of a daily, rather than an hourly temporal resolution, is sufficient to describe contaminant transport. However, when determining the latter portion of the solute breakthrough curve (centre of mass (bulk effect of measures) or the total exit of a contaminant from the profile), an hourly time-step is recommended. While higher quality soil physical data with respect to a specific soil profile, allows better estimation of soil hydraulic parameters, a reduction in data resolution as demonstrated herein may be sufficient in some circumstances for the attainment of reasonably accurate simulations of water and solute movement using numerical models. For example, when the importance of the unsaturated zone within the context of total time lag (unsaturated and saturated) to a receptor is minor, a reduction in the complexity of the soil physical data analysis may be justified. Data complexity is more critical where the source is closer to the receptor. The estimates of vertical time lag (<3 years) through the unsaturated zones of 9 soil profiles in Ireland using Hydrus 1D were similar to the results of previous studies using tracers in similar soil types and meteorological conditions. This indicates the suitability of this modelling approach to such scenarios. Differences in vertical time lag estimated using the full soil water characteristic curve and those excluding the – 15 bar values, which is difficult to measure in the laboratory, were typically small. Exclusion of this value may therefore be justified for this purpose in certain circumstances.

The methods described herein can facilitate future experimental design and elucidation of when (a) initial trends and (b) bulk effects of Programmes of Measures on water quality in vulnerable catchments occur.

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