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5 **A framework for determining unsaturated zone time lags at catchment scale**

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19 **Keywords:** Time lag; Soil; Unsaturated; Water Framework Directive; Nitrate

20 **Abstract**

21 The responses of waterbodies to agricultural programmes of measures are frequently delayed
22 by hydrological time lags through the unsaturated zone and groundwater. Time lag may
23 therefore, impede the achievement of remediation deadlines such as those described in the
24 EU Water Framework Directive (WFD). Omitting time lag from catchment characterisation
25 renders evaluation of management practices impossible. Time lag aside, regulators at national
26 scale can only manage the expectations of policy-makers at larger scales (e.g. European
27 Union) by demonstrating positive nutrient trajectories in catchments failing to achieve at least
28 ‘good’ status. Presently, a flexible tool for developing spatial and temporal estimates of
29 trends in water quality/nutrient transport and time lags is not available. The objectives of the

30 present study were first to develop such a flexible, parsimonious framework incorporating
31 existing soil maps, meteorological data and a structured modelling approach, and to secondly,
32 to demonstrate its use in a grassland and an arable catchment (~10 km²) in Ireland, assuming
33 full implementation of measures in 2012. Data pertaining to solute transport (meteorology,
34 soil hydraulics, depth of profile and boundary conditions) were collected for both catchments.
35 Low complexity textural data alone gave comparable estimates of nutrient trajectories and
36 time lags but with no spatial or soil series information. Taking a high complexity approach,
37 coupling high resolution soil mapping (1:10,000) with national scale (1:25,000)
38 representative profile datasets to < 5 m depth, indicated trends in nutrient transport of 10-12
39 months and 13-17 months throughout the grassland and arable catchments, respectively. For
40 the same conditions, regulators relying on data from groundwater sampling to test the
41 efficacy of the present measures would be delayed by 61-76 months and 46-79 months,
42 respectively. Variation of meteorological datasets enabled temporal analysis of the trends in
43 nutrient transport and time lag estimates. Such a tool could help catchment scientists to better
44 characterise and manage catchments, determine locations for monitoring or mitigation, assess
45 the efficacy of current measures, and ultimately, advise policy makers and regulators.

46

47 **1. Introduction**

48 The European Union Water Framework Directive (WFD) (WFD; 2000/60/EC, OJEC,
49 2000) requires that all waterbodies attain ‘good’ chemical qualitative status (amongst other
50 stipulations) within set reporting periods (e.g. 2015, 2021, 2027). Attainment of this status is
51 attempted through implementation of programmes of measures (POM), such as those
52 described by the Nitrates Directive (EC, 1991), which remediate pollution from agricultural
53 sources via land and fertiliser management strategies. Quality status is determined via
54 environmental monitoring implemented by the Environmental Protection Agency (EPA) in
55 accordance with Annex II of the WFD. In Ireland, POM include the implementation of buffer
56 zones, timing of fertiliser application, and prescribed application rates - derogation to which
57 is critical for attainment of national production goals (Food Harvest 2020 (Dept. of
58 Agriculture, Food and the Marine (DAFM), 2010) and Food Wise 2025 (DAFM, 2015)).
59 However, the inherent delay or ‘time lag’ (Sousa *et al.*, 2013) that surplus nutrients (or other
60 potential contaminants such as heavy metals or pesticides) encounter through subsurface
61 pathways renders correlation between POM efficacy and waterbody status challenging (Cook
62 *et al.*, 2003; Schulte *et al.*, 2006; Bechman *et al.*, 2008; Fenton *et al.*, 2011; Huebsch *et al.*,
63 2013; Van Meter and Basu, 2015). Total time lag (t_T), not including the attenuation of
64 nutrients or other pollutants during transport (Huebsch *et al.*, 2013; Jahangir *et al.*, 2013),
65 may be subdivided into unsaturated (t_u) and saturated (t_s) zone components (Fig. 1) (Fenton *et*
66 *al.*, 2011; Sousa *et al.*, 2013). As the unsaturated zone offers an early indication of trends in
67 water quality concentration and POM efficacy, it is a critical zone to monitor in order to
68 guide the expectations of policymakers and stakeholders (Kronvang *et al.*, 2008; Dworak *et*
69 *al.*, 2005; Wahlin and Grimvall, 2008; Huebsch *et al.*, 2013). Transport of water and solutes
70 through this region may occur relatively slowly through the soil matrix or rapidly as a result
71 of preferential transport through macropores (Keim *et al.*, 2012; Kramers *et al.*, 2012). Matrix

72 flow may present the greatest impediment to the achievement of deadlines, as it indicates the
73 slowest rate of solute flushing from the catchment. Hence, it may contribute to prolonged
74 elevation of solute concentration at an abstraction point or surface waterbody, as opposed to
75 rapidly observed peaks resulting from preferential flow (Mellander *et al.*, 2016). Both
76 pathways can and do occur concurrently within a catchment, but the focus of the current
77 paper is on the matrix component, and where t_u is mentioned hereafter, it is this portion which
78 is referred to. Although the effects of soil properties on t_u are acknowledged as a potential
79 impediment to applied POM (EPA, 2015), no framework exists to assess these limitations
80 and associated timeframes in catchments and sub-catchment areas which are vulnerable to
81 nutrient loss through the soil and groundwater pathway. While biogeochemical attenuation
82 factors are also important (Jahangir *et al.*, 2013; Van Meter and Basu, 2015), the current
83 paper addresses the hydrological component of t_u , which may be differentiated into the
84 following stages: initial breakthrough or trends (IBT/Trend), peak breakthrough (Peak),
85 centre of mass (COM – indicating the bulk effect of POM), and complete exit of the solute
86 from the profile (Exit) (Vero *et al.*, 2014; Fenton *et al.*, 2015). The IBT/Trend is particularly
87 critical as it represents the first instance in which conservative nutrients transported by water
88 may be observed at the base of the soil profile subsequent to implementation, and thereby
89 indicates the general direction of water quality response. IBT/Trend reflects initial effects of
90 POM, as might be ascertained from monitoring networks in the unsaturated zone or shallow
91 groundwater.

92 Numerical models simulate water flow and solute transport in the unsaturated zone
93 (Saxena and Jarvis, 1995; Pang *et al.*, 2000; Pachepsky *et al.*, 2004; Schoups *et al.*, 2008;
94 Konikow, 2011), and can therefore be used to assess t_u (Bouraoui and Grizzetti, 2014). Such
95 models require input data pertaining to soil hydraulic properties (Durner and Lipsius, 2006;
96 Vero *et al.*, 2014; Fenton *et al.*, 2014), temporal meteorological data (Mertens *et al.*, 2002;

97 Gladnyeva and Saifadeen, 2013; Vero *et al.*, 2014) and boundary conditions (Jacques *et al.*,
98 2008; Vereecken *et al.*, 2008). Vero *et al.* (2014) examined the consequences of soil and
99 meteorological input data complexity on t_u estimates produced using the Hydrus 1D model
100 (Šimůnek *et al.*, 2005). Results indicated that low-complexity soil data (textural properties
101 and bulk density (ρ_d)) were sufficient to indicate trend response at the base of a soil profile to
102 POM. Further soil hydraulic parameter evaluation (Fenton *et al.*, 2015) indicated that three
103 popular laboratory textural analyses methods (pipette, laser diffraction and hydrometer)
104 perform equally well as sources of low-complexity data. Previously, Fenton *et al.* (2010)
105 estimated ranges of t_u for Ireland using default values from the literature to simulate the
106 unsaturated and saturated zones. Since then, more extensive soil datasets have become
107 available via the Irish Soil Information System (SIS) (Creamer *et al.*, 2014), and the Irish
108 Agricultural Catchment Programme (ACP) (Wall *et al.*, 2011) is currently testing the efficacy
109 of agricultural POM implemented under the Nitrates Directive. Therefore, the primary
110 objective of the current paper was to develop a parsimonious, readily implementable
111 framework for the estimation of unsaturated soil time lag ranges in agricultural catchments.
112 This framework will provide a mechanism by which catchment scientists can distinguish
113 between various stages of t_u , and hence increase the detail included in projections of time lag
114 trajectories. To fulfil this objective, the current study utilised onsite meteorological (from
115 2012 onwards to match implementation of POM) and soil data (from the Irish SIS) for two
116 agricultural catchments, as inputs to the Hydrus 1D numerical model (Šimůnek *et al.*, 2005).
117 The secondary objective was to examine long-term t_u under future moderate rainfall
118 scenarios, in order to comment on the achievability of subsequent WFD deadlines (e.g. 2021,
119 2027) within these catchments.

120 **2. Materials and Methods**

121 In the development of the modelling framework, the following tasks were performed
122 for both catchments: identification of catchment boundaries using GIS, collation of SIS soil
123 and meteorological datasets, validation of the soil series via a soil survey and auguring
124 campaign, numerical modelling using Hydrus 1D and pertinent hydraulic parameter datasets
125 (ranging from low- to high-complexity soil data and site specificity), and analysis and
126 interpretation of model outputs. Other unsaturated zone numerical models (e.g. VLEACH or
127 STANMOD) may also be suitable for implementation within the current framework.

128 *2.1 Description of the Modelling Framework and Data Sources*

129 The assessment of t_u followed the structure summarised in Fig. 2. The
130 modelling framework consists of a protocol for the selection of input data resolution
131 (meteorological data) and complexity (soil data), identification of appropriate boundary
132 conditions, modelling of vertical water/solute transport and division of the resulting
133 breakthrough curves into markers indicating the various indicative stages of t_u . Simulations
134 were conducted using Hydrus 1D, coupled with appropriate meteorological and soil physical
135 data, and boundary conditions, and resulting breakthrough curves were subdivided in
136 accordance with Vero *et al.* (2014). Many studies have demonstrated the capacity of the
137 Hydrus 1D model to successfully reflect real-life water and solute transport scenarios (Tafteh
138 and Sepaskhah, 2012; Vero *et al.*, 2014; Zeng *et al.*, 2014, amongst others). Model stability is
139 maintained in accordance with Perrochet and Berod (1993). Regarding the meteorological
140 input data (Fig. 2, Step 1), Met Éireann (the Irish meteorological service) operates 25
141 synoptic stations, in addition to over 400 rainfall recording stations (Met Éireann, 2015) from
142 which data may be requested. The ACP also operate weather stations within their study
143 catchments. As indicated by Vero *et al.* (2014), daily or hourly data should be selected based
144 on the stage of t_u in question; for IBT/trend assessment, daily data are sufficient. Atmospheric

145 boundary conditions are applied within the model, to correspond with these meteorological
146 inputs (Jacques *et al.*, 2008).

147 Regarding the soil input data (Fig. 2, Step 2 and Fig. 3), the SIS provides an online
148 national soil map at 1:250,000 scale (Creamer *et al.*, 2014) (<http://gis.teagasc.ie/soils/>). A
149 practitioner may select a map area (the SIS divides Ireland into polygons covering areas of
150 >250 ha) in this database, and will be presented with a number of soil associations likely to
151 occur within this polygon area. A soil association is a mapping unit which aggregates soil
152 types co-occurring within the same landscape pattern. Extracted from a soil association map
153 Simo *et al.* (2016) defined a soil textural map of Ireland, based on the dominant textural class
154 for the lead soil type of the soil association. Within the current study, clips of the catchment
155 areas were obtained from the soil texture map (Simo *et al.*, 2016) to derive a low-complexity
156 soil texture class for each study catchment (Fig. 3, approach I). Hence, generic t_u estimates
157 may be produced based on these data alone (Vero *et al.*, 2014) (Fig. 2, Step 2 – 1st option).
158 The database associates each soil series with ‘modal soil profiles.’ These profiles describe the
159 pedological characteristics that are considered representative of each series within a soil
160 association. Modal profiles indicate horizon-specific characteristic data, including particle
161 size distribution and ρ_d information, from which soil hydraulic parameters can be derived *via*
162 pedotransfer functions (PTF) (e.g., ROSETTA) (Schaap *et al.*, 2001). Moving from the
163 generic soil association approach (indicating a single textural class for the entire profile
164 depth) to the modal profile approach (indicating horizon-specific soil characteristics) (Fig. 2,
165 Step 2 – 2nd option, Fig. 3, approach II) allows the influence of both vertical and horizontal
166 heterogeneity of soil properties to be considered (Mohanty and Zhu, 2007). It is important to
167 note that areas defined by polygons do not necessarily correspond to surface- or groundwater
168 hydrological catchments. In order to derive soil data for specific catchment or sub-catchment
169 areas, it is therefore necessary to transpose the outline of the area in question onto the SIS

170 map using GIS (ArcGIS version 10.2) – as in the study catchments of the current study. This
171 degree of site characterisation corresponds to the soil series mapping approach shown in Fig.
172 3. To increase the resolution of the soil type delineation, validation via ground-truthing was
173 conducted. This involved identification of priority areas within each catchment (determined
174 from landscape, proximity to receptors and soil association borders, etc.). Soil auguring and
175 series identification was then performed in these areas in accordance with Creamer *et al.*
176 (2014). This represents approach III depicted in Fig. 3, and is the highest level of site
177 characterisation.

178 Lower boundary data (Fig. 2, Step 3) is determined according to either known or
179 assumed watertable or bedrock depths. The hydraulic properties of unsaturated bedrock
180 cannot be quantified using the PTF approach, and so only the soil component of the
181 unsaturated zone may be accounted for. It is acknowledged that the full depth to groundwater
182 may include unsaturated bedrock. Where the watertable is deeper than the soil/bedrock
183 interface (i.e. no part of the soil profile is saturated), a free drainage lower boundary
184 condition should be imposed. This condition assumes that water and solute outflow at the
185 base of the profile is unimpeded. As soil pits are not typically excavated to bedrock due to
186 safety concerns and practical challenges, the bottom-most surveyed soil horizon is assumed
187 to account for the remainder of this region, unless geophysical data (if available) indicate
188 otherwise. This assumption reflects the increased homogeneity observed in deep soil horizons
189 (e.g. C horizons), which are less subject to the weathering, biological and management
190 practices which influence shallower horizons, and more closely resemble the parent material
191 (van Breemen and Buurman, 2002). For example, a soil pit is excavated to a depth of 1.8 m,
192 and the bedrock interface is assumed at a depth of 2.5 m. The profile built within Hydrus
193 should equate to 2.5 m in depth, with the properties of the bottommost horizon extrapolated
194 across this unaccounted-for region. Where no data are available, indicative bedrock depths

195 may be identified from geophysical survey, or generic depths may be used. Within the
196 context of Irish environmental policies, it is appropriate to use depths corresponding to the
197 subsoil thickness vulnerability rating depths (3, 5 or 10 m) (DELG, 1999). Where the
198 watertable is shallower than the bedrock, a fixed pressure head may be imposed at the base of
199 the simulated soil profile. A variable pressure head may alternately be applied, although this
200 requires additional data pertaining to watertable depth fluctuations at a similar resolution to
201 the meteorological input data. There are three approaches by which watertable depths may be
202 derived: a) assume generic depths e.g. 0.5, 5 or 10 m (Fenton *et al.*, 2011), b) estimate depths
203 based on landscape position, or c) groundwater monitoring wells. While greatest temporal
204 and spatial accuracy is obtained via monitoring wells, they may not be readily available in
205 many catchments, and so a landscape position approach may be preferred.

206 *2.2 Implementation of the modelling framework in two study catchments*

207 The two study catchments (Grassland and Arable) have been previously investigated as part
208 of the ACP (Fealy, 2010; Mellander *et al.*, 2012; ACP, 2013; Mellander *et al.*, 2014;
209 Mellander *et al.*, 2016). Site summaries are presented in Table 1, and SIS association maps
210 (Creamer *et al.*, 2014) (derived from the online resource) are available as supplementary data.

211 *2.2.1. Meteorological data*

212 Two modelling exercises were conducted, using separate meteorological datasets. In
213 the first exercise, t_u at the study sites was estimated in response to POM applied in 2012 (as
214 in the Irish scenario) at each site, and so to comment on the 2015 reporting period, a 3-yr
215 daily meteorological dataset (rainfall and evapotranspiration) was obtained from onsite
216 weather recording stations. As this study was conducted in 2015, data for that year were
217 incomplete and so omitted; data spanned from 1st January 2012 to 10th December 2014. In the
218 second exercise, an example year, 1991, having median rainfall (865 mm), evapotranspiration

219 (443 mm), and hence effective rainfall (ER) (422 mm) values, and exhibiting stereotypical
220 annual rainfall patterns, was selected (due to its moderate meteorological conditions), and
221 duplicated to provide a 13-yr dataset of moderate meteorological conditions, by which long-
222 term simulations were conducted.

223 2.2.2. *Soil Data*

224 The SIS online database was used to obtain soil association, subgroup and series data by
225 overlaying the outline maps of the two study catchments on the SIS map using GIS
226 (supplementary data). Horizon-specific data (particle size distribution and ρ_d) for each of the
227 modal profiles were processed using ROSETTA (Schaap *et al.*, 2001) to derive soil hydraulic
228 properties *via* PTF. Hydraulic parameters are available as supplementary data.

229 2.2.3 *Boundary data*

230 Interpretation of ground penetrating radar (GPR) was used to estimate bedrock depths
231 along two hillslope transects in each catchment. Hence, maximum and minimum profile
232 depths were determined (Mellander *et al.*, 2014). For the grassland site, four soil depths were
233 simulated (0.5, 3, 5 and 10 m), while three depths were simulated at the arable site (1, 3 and 5
234 m). At the grassland site, the shallowest depths correspond to near-stream or low-slope
235 positions, in which the watertable was present within the soil profile, while the deeper
236 scenarios reflect mid- or upslope positions. At the arable site, GPR revealed undulating
237 rockhead along the hillslope. Consequently, slope position and distance from the receptor
238 cannot be correlated to depth of the soil profile, and each scenario may occur at various slope
239 positions.

240 3. Results and Discussion

241 3.1 *Catchment Mapping and Soil Parameters*

242 Soil association maps of the grassland and arable catchments, respectively, are
243 available as supplementary data. The broad textural class of both catchments is loam, and
244 both are dominated by the Ballylanders series, and in the arable catchment – the highly
245 similar Clonroche series (Table 2). The arable site exhibits a greater total diversity of series
246 (Mellander *et al.*, 2014), however, many of these series represent a very minor proportion of
247 the total catchment and so may not be indicative of the dominant hydrological behaviour of
248 the area (e.g. the Duarrigle and Kilrush series represent only 1% and 3% of the arable
249 catchment, respectively). The relative area represented by each soil series in each catchment
250 is shown in Table 2. Extensive characterisation of these study catchments in conjunction with
251 the ACP rendered this possible; however, for most Irish catchments, further soil survey
252 (auguring campaigns) would be required. This information is helpful in determining which
253 modal profiles exert the greatest control over t_u within a catchment. However, even without
254 such information, the ranges of t_u are indicative of overall catchment behaviour. In the
255 absence of this high level of characterisation, the modelling framework may be implemented
256 in accordance with the second approach depicted in Fig. 3, and that these data only lend
257 context to model results. In some circumstances, for example the grassland catchment,
258 preliminary high resolution mapping coupled with targeted field survey, suggests greater
259 complexity than that suggested by the SIS maps (Murphy *et al.*, 2015). Apropos to the
260 objective of integrating soil and meteorological data at the available scales, as inputs to a
261 modelling framework for t_u assessment, the approach herein is effective in establishing
262 catchment-specific temporal ranges using only existing available data-sources. With respect
263 to catchment scale and practicalities regarding national implementation, use of SIS (or similar
264 1:25,000 scale soil maps) presents as optimum, with the caveat that refining to the 1:10,000
265 scale may be desirable where a high degree of characterisation is required.

266 The dominant series in both catchments were brown earths, and exhibited similar
267 characteristics, although in the arable catchment, minor series exhibited a greater diversity of
268 hydraulic properties. This implies that certain areas within a catchment may exhibit unique
269 hydrological behaviours, which are consistent with the critical source area concept (Pionke *et*
270 *al.*, 2000; Galzki *et al.*, 2011; Shore *et al.*, 2014; Thomas *et al.*, 2016), and which may be
271 identified via catchment characterisation approaches (e.g. those described by Packham *et al.*,
272 2013). Implementation of the methodological framework described herein may thus be
273 targeted towards specific areas within a catchment identified by these approaches as prone to
274 exhibit prolonged t_u .

275 3.2 Time Lag Estimates – 2012 implementation

276 Results of the modal profile simulations subsequent to 2012 POM implementation
277 scenario are shown in Table 2. The IBT/trends at the base of the soil profile were observed
278 between 1 to 27 months, and 3 to 17 months depending on profile depth, for the grassland
279 and arable sites, respectively. The wider range in IBT/trend observed in the grassland
280 catchment reflects the depth of the soil zone, which exceeded that of the arable catchment.
281 Exit of the solute was only achieved at shallow depths in either catchment (7-25 and 15-24
282 months, for grassland and arable, respectively) within the three-year simulation period. For
283 deeper profiles, total exit of the solute from the soil was not achieved. Differences in t_u within
284 either catchment was greater for the latter markers (COM and Exit), but IBT/Trend ranged
285 between 14-26 months, depending on soil depth. This suggests that identification of the area
286 represented by each soil series within a catchment is of greater importance where the soil is
287 deeper (in upslope positions), or when solute exit, rather than trends, is the primary interest. It
288 must be considered that in both study catchments, the prevalent soil series represent a
289 relatively small range of soil types (brown earths). In catchments exhibiting more diverse
290 soils, the differences between series are likely to be greater. Taking a lower-complexity

291 textural class approach (Fig. 3 – Approach I) indicated IBT/trends in 0-24 months and 1-13
292 months, for the grassland and arable catchments, respectively, depending on profile depth.
293 While these ranges roughly agree with those determined via the modal profile approach (Fig
294 3. – Approach II and III) and may be useful for generally approximating catchment
295 behaviour, they are implicitly less informative than the modal profile approach. Selection of
296 the appropriate approach should therefore, be informed by the degree of characterisation
297 required and data availability.

298 It is important to note that rapid groundwater response to agricultural practices may
299 also be observed due to preferential flow, particularly on soils exhibiting high macroporosity
300 (Keim *et al.*, 2012; Kramers *et al.*, 2012). For catchments (or sub-catchment regions) in
301 which such soils predominate, t_u is unlikely to prevent attainment of WFD deadlines, hence,
302 assessment using the present framework is unnecessary and not recommended. A user may,
303 however, wish to model such soils using appropriate model settings (dual-
304 porosity/permeability). As the focus of the current paper is on the prolonged aspects of t_u ,
305 approaches to preferential flow modelling are not discussed in detail herein. However, some
306 guidance as to the identification of those latter scenarios is beneficial. Vervoort *et al.* (1999)
307 noted that quantification of the relationship between the structure of a soil and its propensity
308 for preferential flow is challenging – visual assessment or cracks and biopores, dye tracer
309 tests (Kramers *et al.*, 2012), tomography (Bacher *et al.*, 2015) and inverse modelling (Arora
310 *et al.*, 2011) have all been successfully used; however, these require access to the soils in
311 question, which may not be feasible where existing quantitative map data (such as from the
312 SIS) are relied upon. Morphological characteristics included in map or soil survey data may
313 provide useful qualitative indicators. Profile or horizon characteristics such as aggregation
314 (Quisenberry *et al.*, 1993), structure and landscape position (Vervoort *et al.*, 1999), can
315 suggest tendencies towards preferential flow. At a catchment scale, soil-based hydrologic

316 classification systems, such as the UK's HOST (Boorman *et al.*, 1995) may also be
317 employed. Although it is beyond the scope of the present research to integrate preferential
318 flow to the framework, this aspect recommends itself as a prime area for further research and
319 development.

320 The results (Table 2) demonstrate that a single t_u figure cannot quantify the range of t_u
321 durations exhibited across a catchment, with varying soil series and water-table depths.
322 Hence, remediation of water quality from applied mitigation strategies may not be directly
323 observable where specific areas within a catchment are transmitting solutes over a prolonged
324 period, despite flushing in shallower or more rapidly drained regions. This is consistent with
325 Mellander *et al.* (2015), who reported temporal and spatial variation in groundwater response
326 in these catchments. Regarding the initial 2015 WFD deadline, these results indicate that
327 assuming implementation of POM at a latest date of 2012, achieving full effects (indicated by
328 Exit) within this timeframe is unrealistic, even when t_s is omitted. While this result is
329 consistent with earlier research (Fenton *et al.*, 2011), the current framework offers the
330 advantage of differentiating between the various stages of t_u . In particular, assessment of
331 trend response better informs policy decisions relating to POM efficacy in the immediate
332 future.

333 *3.3 Time Lag Estimates – Long-term simulations*

334 The results of long-term simulations, using a moderate meteorological dataset, are
335 shown in Table 2 (representing the Exit stage only). For the grassland site, long-term t_u
336 (indicating complete effect of POM) exceeded 100 months/8 yr in deep profiles. Even under
337 moderate profile depths (3-5 m) (likely at mid-slope positions), Exit ranged from 42 to 63
338 months (3.5-5 yr). In the arable catchment, maximum long-term t_u was less than that
339 observed in the grassland catchment, and ranged between 46 and 79 months (3 to *c.* 6.5 yr),

340 due to the relative shallowness of the soil profiles. This demonstrates that depth of the soil
341 profile is a critical control on t_u ranges, and geophysical data should be preferred over generic
342 values, particularly where groundwater quality is of poor or declining status.

343 These results indicate that even under moderate meteorological conditions, for many
344 soil depths, it may take in excess of a 6-yr reporting period for the full effects of POM to be
345 observed at groundwater, with a subsequent delay imposed by t_s prior to marked changes at a
346 surface water receptor or abstraction point. While this is a relatively simplistic approach to
347 meteorological scenario testing, the results are indicative of the timeframes in which t_u
348 operates, and in which policy and subsequent evaluation of POM efficacy should be
349 designed. Specific meteorological factors that should be considered in future scenario testing
350 include the intensity and timing of precipitation, as these directly influence t_u and
351 subsequently, t_s . Wendroth et al., (2011) correlated depth of leaching of bromide (which is
352 frequently used as a proxy for conservative solutes such as nitrate) at a field scale with the
353 proximity of precipitation events to solute application. The degree of influence exerted by
354 meteorological conditions, land use or soil parameters on leaching rates varies by depth.
355 Yang *et al.* (2013) revealed that t_u in the upper soil horizons (<10 cm) is dictated primarily by
356 rainfall intensity, while the timing of solute application is the dominant factor in the
357 subsequent horizon (10-20 cm), and soil physical parameters becoming the increasingly
358 important drivers deeper within the profile. These results should guide model users as to the
359 importance of meteorological versus soil input data, depending upon the depth of the soil in
360 question.

361 Assuming the scenario whereby POM were implemented by the end of 2012, trends
362 should be observed within the first reporting period in both catchments. However,
363 considering COM as an indicator of the bulk effect of POM (Vero *et al.*, 2014), it is towards
364 the latter stages of the first reporting period that substantial changes in groundwater quality

365 are expected. Temporal trend analysis may therefore, be a more useful and informative
366 indicator of POM efficacy. As indicated by Vero *et al.* (2014), the saturated approach of
367 Fenton *et al.* (2011) is useful as an indicator t_u ; however, it cannot distinguish between the
368 various stages (IBT/Trend, Peak, COM, Exit) and so provides a general description only. The
369 results of that paper (under ER conditions of *c.* 800 mm yr⁻¹ and n_e of 40%) are in good
370 agreement with the results presented here. Exit of the solute from the soil (potentially
371 challenging to discern *via* monitoring due to low concentrations) approached or exceeded 72
372 months/6 yr for many soil series and profile depths. This indicates that although the reporting
373 periods suffice for trend assessment, they are too short to observe the full effects of POM.
374 Although these temporal results may be considered unsurprising in light of the existing
375 literature, the utility of this modelling framework is in incorporating both an input data
376 decision support system and a structure for breakthrough curve analysis into an integrated
377 system. Using this system, a model user can maximise the utility of their available data
378 within the context of the stage of solute transport with which they are concerned.

379 While it is not within the scope of this paper to indicate t_s and hence, t_T , the similarity
380 between the results herein and those of Fenton *et al.* (2011) suggest that their assertion of
381 remediation timeframes between 2019 and 2033, depending on unsaturated zone depth and
382 proximity to receptor, are realistic. While estimates produced under the saturated assumption
383 provide a useful first estimate of t_u , they produce only a single figure, and cannot differentiate
384 between the various stages of solute breakthrough, unlike the framework presented herein,
385 which provides a more comprehensive description of t_u . Regarding t_s , transition zone
386 delineation consistency and thickness, bedrock type, thickness and degree of fracturing
387 controls the duration of this component of t_T . Within the Irish context, preliminary estimates
388 of minimum t_s (contingent upon k_s and specific yield) over a distance of 500 m ranged
389 between 0.06 and 6.85 years (Fenton *et al.*, 2011). However, it is important to note, that these

390 are minimum values, and will be exceeded in many catchments. Further research into the t_s
391 component and methodologies for its assessment are forthcoming.

392 *3.4 Implications for policy and monitoring*

393 That t_u should preclude attainment of WFD deadlines is not new; Fenton *et al.* (2011)
394 indicated this in advance of the first reporting period. The utility of this framework lies in its
395 ability to disentangle the various stages of t_u , and, based upon the areas represented by a
396 specific soil series, to anticipate the overall trends likely to be observed within a catchment
397 over the forthcoming reporting periods. Hence, catchment scientists can provide
398 policymakers with early indicators of likely trends and responses to mitigation measures
399 through the judicious use of existing data. This removes time lag from the category of
400 ‘generic excuse’ (Scheure and Naus, 2010), by adding both spatial and temporal specificity.

401 Thomas *et al.* (2016) used a digital elevation model (DEM) to define and map CSAs
402 for nutrient loss via overland flow. Those same maps may be also used to inversely identify
403 those areas which are prone to persistent, low concentration nutrient transport due to vertical
404 transport through the unsaturated zone. This information is valuable in determining which
405 areas within a catchment should be targeted for the implementation of mitigation or
406 remediation techniques, which has implications for their efficacy and cost-effectiveness. It
407 should further be noted that in line with the functional land management concept (Schulte *et*
408 *al.*, 2014; Coyle *et al.*, 2016), a soil fulfils multiple functions, one of which is water
409 purification. Understanding t_u durations alone does not account for subsurface
410 transformational processes e.g. denitrification (Seitzinger *et al.*, 2006; Green *et al.*, 2009;
411 Jahangir *et al.*, 2013). Saturated hydraulic conductivity of soils/subsoils/bedrock have been
412 correlated with nitrate concentration and N_2/Ar ratios at field scales (Fenton *et al.*, 2009;
413 Fenton *et al.*, 2012) and indeed at landscape scales (Jahangir *et al.*, 2012). Therefore, an
414 understanding soil type and soil physical parameters can guide not only time lag estimates at

415 catchment scale but also provide appropriately scaled information required for translation
416 into environmental policy, in accordance with the DPSIR (drivers, pressures, states, impacts
417 and responses approach (Bouma and Droogers, 2007).

418 Mapping endeavours (e.g. Creamer *et al.*, 2014) demonstrate that a variety of distinct
419 soil series may be observed within a single catchment, and so a specific slope position may
420 exhibit one of several different t_u durations, dependant on which soil series is present. For
421 example, in the arable catchment, the range of soil series and the undulating depth to bedrock
422 (3 m to 5 m) across the entire slope, indicates up to ten different t_u durations. Therefore, a
423 range of potential t_u (for each marker: IBT/Trend/Peak/COM/Exit) provides a more realistic
424 tool to assess timescales within a catchment. Analysis of trends in water quality response to
425 POM is inherently limited by spatio-temporal factors; namely, the position of monitoring
426 points within the landscape and the stage of time lag which may be assessed at those
427 locations. For example, surface-water quality is influenced by the sum of all hydrological
428 processes in the catchment, including surface run-off, lateral subsurface flow, baseflow etc.
429 Consequently, it is challenging to disentangle the trend effects of recent POM from the
430 legacy of past practices, or those effects arising from measures implemented in different parts
431 of the catchment. Likewise, monitoring of groundwater will indicate chemical concentrations
432 reflective of both past and present measures, and at low-slope positions, will be subject to the
433 import of water/contaminants from higher along the transect. As such, monitoring of
434 waterbodies represents t_T , or t_u plus some portion of t_s , and cannot discriminate between the
435 components of time lag (saturated versus unsaturated), or its various stages
436 (IBT/Peak/COM/Exit). Unsaturated zone modelling according to the present framework
437 enables trends at the base of the soil profile to be determined independently of confounding
438 influences. This provides an earlier indication of trend responses than is possible via
439 monitoring of ground- or surface-waters. Considering both ranges and stages of t_u may, with

440 further research, facilitate examination of the potential for nitrate attenuation and dilution in
441 the subsurface. For example, prolonged t_u may suggest greater attenuation than is likely in
442 more rapid profiles. Conversely, where a catchment is dominated by very shallow soil
443 profiles, or by overland flow pathways, long term t_u values are less informative, and
444 attenuation potential may be lower. Such theories present as important areas for further
445 research.

446 **Conclusions**

447 The results of this study indicate a range of potential unsaturated time lag within each
448 catchment, depending on the stage of transport in question, soil series, and depth of the soil
449 profile (or slope position). In the study catchments, trends were first observed at the base of
450 the soil profile up to 27 months subsequent to the 2012 implementation of POM scenario,
451 while the full effects may exceed 11 and 6 yr within the grassland and arable catchments,
452 respectively. These lags should be considered as long, in light of the 6-yr reporting period
453 cycles defined by the WFD. Under a scenario whereby POM implementation occurred in
454 2012, the 2015 deadline therefore allowed an insufficient period of time to bear full effect on
455 water quality. However, based on the long-term simulations, response at groundwater should
456 be observed at these sites within the subsequent reporting period (2021). This basic modelling
457 framework can, in future, be built upon in order to account for additional delay due to
458 nutrient attenuation and may be integrated with other tools for the characterisation of
459 catchment hydrology.

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Figures

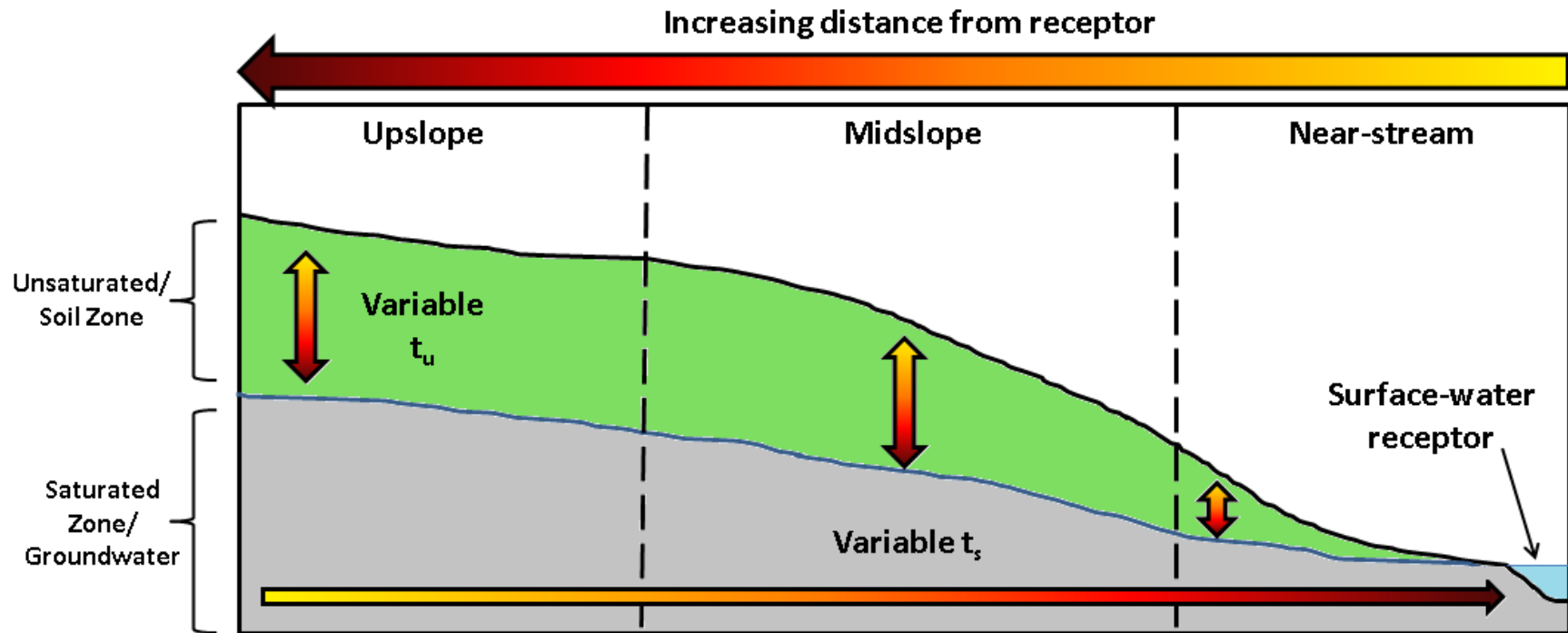


Fig. 1: Total time lag (t_T) from source to receptor, including the unsaturated soil pathway (t_u) and the saturated groundwater pathway (t_s). Arrows indicate the variable duration of t_u and t_s , depending on the depth of the soil profile and proximity to a receptor, respectively.

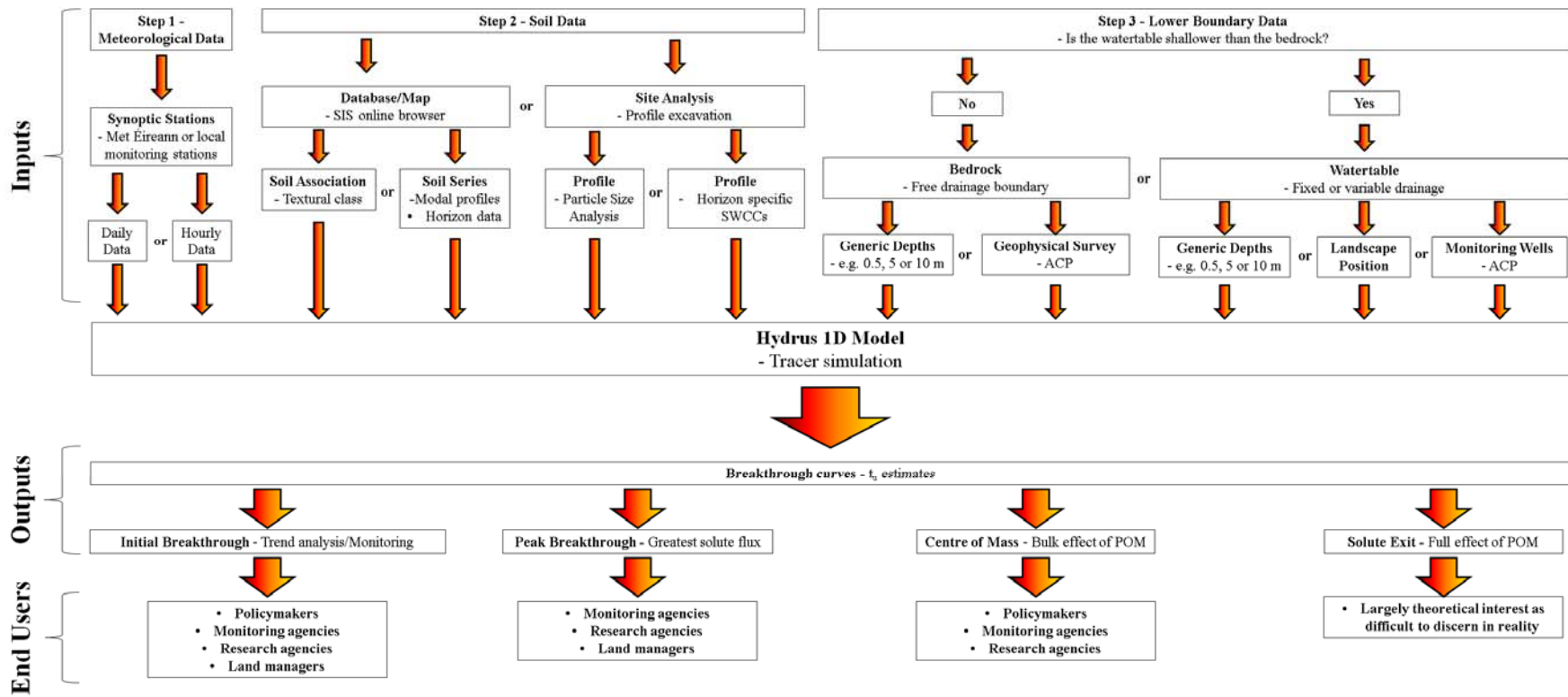


Fig. 2: Modelling framework for assessment of unsaturated zone time lag, including data-sources and outputs. Input data complexity within each step is increased by moving from left to right. Step 2 is further developed in Fig. 3.

Mapping Approaches

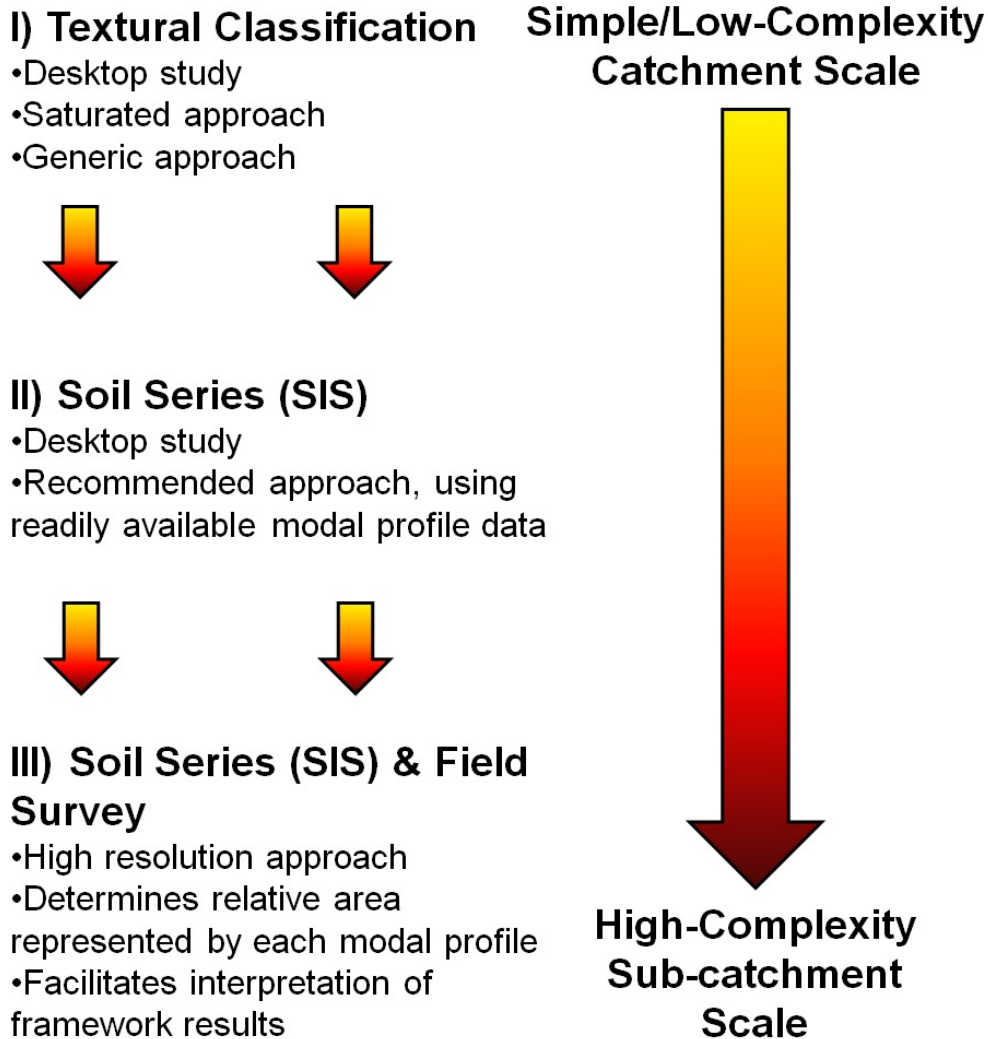


Fig. 3: Schematic of the catchment soil mapping approaches, from desktop to field survey. Increasing the complexity (by moving from top to bottom) aids in interpretation and contextualisation of results. These approaches correspond to Stage 2 in the time lag framework (Fig. 2). Maps of the grassland and arable catchments corresponding to each approach are available as supplementary materials.

Tables

Table 1: Summary of Grassland and Arable characteristics. Rainfall data was obtained from the nearest Met Eireann synoptic stations (Johnstown Castle and Cork, respectively).

	Grassland	Arable
Area (ha)	758	1,117
30-Year (1989-2020) Average Rainfall (mm)	1228	1060
Dominant Soil Permeability	Moderate	High
Dominant Subsoil Permeability	High	High
Bedrock Permeability	High	Low
Unsat. Soil Depth (m)	0.5 – 10	1 – 5
Dominant pathway	Subsurface	Subsurface

Table 2: Results of modal profile simulations, subsequent to 2012 implementation, according to various profile depths indicative of slope position. X indicates failure to achieve marker within simulation period and t_u (unsaturated zone time lag) is reported in months.

Site	Association	Series	Area %	Depth m	Breakthrough (months) (subsequent to 2012 implementation)				Moderate Rainfall Conditions	
					IBT/Trend	Peak	COM	Exit	Long-term t_u	Saturated t_u
Grassland	Ballylanders		50	0.5	1	3	3	7	13	4
				3	6	11	12	25	46	48
				5	11	16	X	X	63	80
				10	22	X	X	X	104	160
	Rosscarbery		34	0.5	<1	1	3	7	12	8
				3	6	11	11	24	42	46
				5	10	15	19	3	61	77
				10	20	32	X	X	100	155
	Driminidy/ Newport		16	0.5	1	2	3	7	12	6
				3	7	12	14	25	51	38
				5	12	22	X	X	76	64
				10	27	X	X	X	132	127
Arable	Ballylanders		75	1	4	7	8	15	22	15
				3	9	14	X	X	23	46
				5	13	27	X	X	46	77
				1	4	8	9	22	24	14
				3	10	16	X	X	48	42
				5	14	28	X	X	66	69
	Duarrigle	1	1	3	7	9	24	25	12	
			3	11	22	X	X	55	37	
			5	16	33	X	X	78	61	
	Kilpierce	7	1	4	8	9	24	26	13	
			3	11	22	X	X	55	39	
			5	16	X	X	X	78	65	
	Kilrush	3	1	5	8	9	16	22	10	
			3	11	24	X	X	54	31	
5			17	X	X	X	79	52		
Other		14	Series representing minor land area							

