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Predicting microbial water quality with models: Over-arching questions for managing risk in agricultural catchments

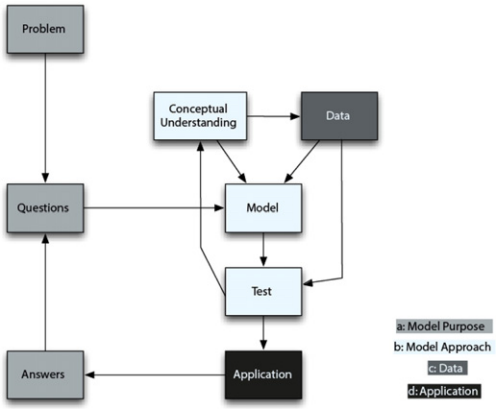
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HIGHLIGHTS

- 4 overarching questions identified to guide modelling of catchment microbial dynamics
- Model purpose, modelling approach, data availability & model application are debated
- Awareness & respect for different FIO modelling approaches is important
- Short & longer-term research priorities for more effective FIO modelling are proposed

GRAPHICAL ABSTRACT



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ABSTRACT

The application of models to predict concentrations of faecal indicator organisms (FIOs) in environmental systems plays an important role for guiding decision-making associated with the management of microbial water quality. In recent years there has been an increasing demand by policy-makers for models to help inform FIO dynamics in order to prioritise efforts for environmental and human-health protection. However, given the limited

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evidence-base on which FIO models are built relative to other agricultural pollutants (e.g. nutrients) it is imperative that the end-user expectations of FIO models are appropriately managed. In response, this commentary highlights four over-arching questions associated with: (i) model purpose; (ii) modelling approach; (iii) data availability; and (iv) model application, that must be considered as part of good practice prior to the deployment of any modelling approach to predict FIO behaviour in catchment systems. A series of short and longer-term research priorities are proposed in response to these questions in order to promote better model deployment in the field of catchment microbial dynamics.

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1. Introduction

Determining the microbial quality of recreational, drinking, irrigation and shellfish-harvesting waters is important to ensure compliance with health-related standards and associated legislation. Levels of microbial pollution in environmental matrices are often measured by quantifying faecal indicator organisms (FIOs). FIOs (e.g. *Escherichia coli* and intestinal enterococci) play a significant global role in informing regulators and environmental managers of levels of faecal pollution and hygienic status of water resources. For example, in the European Union, FIOs are key parameters monitored within the Bathing Water Directive (BWD) (CEC, 2006a) and Shellfish Waters Directive (CEC, 2006b) to regulate microbial water quality in protected areas. In the USA, FIOs are monitored under the Clean Water Act, and pathogen indicators (predominantly *E. coli*) are the leading cause of watercourse impairment (USEPA, 2015). The microbial quality of irrigation water and implications for food safety is also gaining increased recognition (Pachepsky et al., 2011) particularly in the USA after the Food Safety Modernization Act was signed into law in 2011. In New Zealand, the National Policy Statement for Freshwater Management (NPS-FW, 2014) plays a pivotal role in driving an agenda for delivering better national water quality. The NPS-FW (2014) includes a National Objectives Framework, which sets out water quality standards and "national bottom lines" which are minimum standards that all waters in NZ should comply with. One of these national minimum standards relates to *E. coli* concentrations in all waters.

Historically most research into waterborne disease has focused on human faecal sources such as sewage and storm-water (McBride et al., 2013). However, there is a growing recognition that animal faeces also represent a significant human health risk (Soller et al., 2015; Dufour et al., 2012; Till et al., 2008). Human faecal sources are generally easier to manage 'point' sources from sewage systems, while agricultural sources are the more difficult to manage 'diffuse' sources (Vant, 2001). Some of the challenge of managing these faecal sources comes from a range of ownership issues. For example, in a large catchment there may be a number of point sources of human faecal discharge to a river but the management of this may be the responsibility of only one or a few municipal authorities or sewerage undertakers that have clear responsibility for water quality management and/or public health. In contrast, sources of animal faeces will be the responsibility of (a) the many farmers who manage domesticated animals and (b) different government (or quasi-government) departments for the management of wild animals (e.g. water fowl, deer, and beavers), neither of which have water quality or public health as a prime responsibility. Catchment regulators implementing, for example, the EU Water Framework Directive (2000) or the US Clean Water Act are therefore faced with a complex system for multiple sources of diverse sanitary significance. To make sense of, and to support decision-making on, multiple sources of faecal material discharges from a range of different activities we need catchment scale models that can fairly apportion water quality risks to individual contaminant sources.

The application of catchment models to predict microbial water quality, coupled with direct detection and quantification, plays an important role for guiding decision-making associated with the management of water resources. Recent examples of model applications to inform environmental management of FIOs include the use of catchment screening tools to determine FIO source apportionment at bathing waters according to land use (Kay et al., 2010), development of farm-scale indexing approaches to elucidate FIO risks arising from different farm practices (Muirhead, 2015), and the simulation of *E. coli* persistence in cowpats to help further our understanding of population dynamics of FIOs on grazed pastures (Martinez et al., 2013). However, modelling the fate and transfer of FIOs at different spatial scales poses a considerable challenge to the research and policy community (Oliver et al., 2009; Coffey et al., 2007; Pachepsky et al., 2006). This is because our level of understanding of FIO behaviour in the environment is still relatively poor compared to other agricultural pollutants such as phosphorus (P) and nitrogen (N) (Oliver et al., 2015; Kay et al., 2008a). The persistence of FIOs in the environment is highly context specific and the modelling of FIOs in agricultural catchments therefore presents a different set of challenges to P and N. This set of challenges includes their potential to replicate and increase in number under favourable environmental conditions, or experience population die-off at varying rates depending on a range of unfavourable biotic and abiotic factors (Stocker et al., 2015). Thus, it is critical that we try to understand the survival, transfer and export of FIOs better once they are excreted into the wider environment, because improved knowledge and data on the behavioural characteristics of these micro-organisms will enhance our ability to model and predict their interactions with, and responses to, the world around us (e.g. Oliver et al., 2015; Guber et al., 2015; Quilliam et al., 2014; McKergow and Davies-Colley, 2010; Wyer et al., 2010; Kay et al., 2008b; Muirhead et al., 2004). To address the gaps in our current understanding, some of the key research questions under investigation by the research community include:

(i) how do the hydrological pathways that connect FIO sources to water bodies vary in space and time across different catchment types and how does this impact on FIO travel times through the environment?;
(ii) to what extent does the probability of FIO die-off vary for different environmental conditions (in different environmental matrices) around the world?;
(iii) how do we integrate FIO behavioural characteristics (e.g. their ability to persist or move in the environment) into model frameworks that are useful for decision-makers?;
(iv) how will the export of FIOs from the landscape alter under projected climate change and/or land use change?

Answers to these questions rely on a combination of laboratory, field and modelling approaches and will take time to mature. Furthermore, it is well recognised that the quality of modelled outputs has an implicit reliance on the quality of the field and laboratory data used to populate each model (de Brauwere et al., 2014). With microbial water pollution generating increased attention through, for example, tightening of the BWD standards in Europe (Quilliam et al., 2015) and FIOs being recognised as the leading cause of watercourse impairment in the USA, there is an increasing demand by policy-makers for models to help inform catchment microbial dynamics in order to prioritise efforts

for environmental and human-health protection (Coffey et al., 2015). Given the limited evidence-base on which FIO models are built relative to other agricultural pollutants (e.g. nutrients) it is therefore imperative that the end-user expectations of FIO models are appropriately managed by model developers. In response, this commentary highlights four over-arching questions that must be considered as part of good practice prior to the deployment of any modelling approach, irrespective of their geographic application in the world, to predict FIO behaviour in catchment systems. In turn, these questions link to a series of short and longer-term research priorities to enable more effective FIO modelling.

2. Over-arching rationale to guide development of FIO modelling in catchments

Models are often used to help answer research or policy-orientated questions. Fig. 1 depicts a generic modelling process used to generate answers (and new questions) to environmental problems. We use this generic process as a template to discuss modelling challenges associated with FIOs. The modelling process can be broken down into four core components, namely: 'model purpose', 'model approach', 'data' and 'application'. Individually, each component of the modelling process will accommodate a range of requirements for fundamental research to improve our wider understanding of FIO fate and transfer. However, taken together they provide an integrated and iterative approach to microbial fate and transport model development. The four modelling components, each coupled with a higher level question, are discussed below. We argue that an internationally relevant framework of over-arching questions is both timely and important to steer future laboratory and field-based research in order to underpin and improve our modelling capability in the rapidly developing field of catchment microbial dynamics. Rather than contributing in-depth discussions to an already overcrowded literature of comprehensive FIO and pathogen modelling reviews this commentary aims to provide a more critical focus for future research direction, enabling more effective deployment of models for predicting water quality in agricultural catchments.

2.1. Model purpose: what is the question we want to answer?

Irrespective of environmental context or pollutant, no model can be developed to predict everything, everywhere, all of the time. Yet, end-users often misunderstand a model's predicative capability, or apply it inappropriately (Dickey-Collas et al., 2014) thus limiting its predictive capability. Both misapplications can be avoided by assessing a model's purpose and clarifying its expected outputs, defining the question of interest then determining whether a particular model can answer it.

The prediction of FIO behaviour in the environment can be undertaken for a number of reasons. For example, to: (i) explore real-time prediction of microbial pollution in recreational waters; (ii) model the dynamics of short term pollution incidents in the aquatic environment; (iii) understand the contributions of FIOs delivered to receiving waters via different hydrological pathways to inform mitigation and management; (iv) enable screening to guide regulators and/or policy-makers in prioritising decisions; (v) predict future scenarios due to climate or land-use change; or (vi) test new hypotheses to understand an environmental system better and advance our knowledge further. Recognising that no single model can inform all of these objectives is crucially important. End-users have a responsibility to ensure that they understand a model's purpose prior to its application. Model developers have a responsibility to be transparent about their model's strengths and limitations and to not promote model acceptance irrespective of end-user needs.

Model purpose and scale are intricately linked, and appreciating the acceptable range of scales at which a model can operate effectively is essential for robust prediction. There are significant questions concerning the extent to which FIO responses and behaviour observed and quantified on the microscale can be extrapolated to reflect behaviour at the catchment scale. This challenge is not restricted to microbial pollution and there are opportunities to learn from other research disciplines (e.g. nutrient management) (Vermeulen et al., 2015). Demand for models capable of predicting pollutant flux in catchment systems is increasing in part due to policy drivers that require assessments of how changes in management might impact on water quality in the future

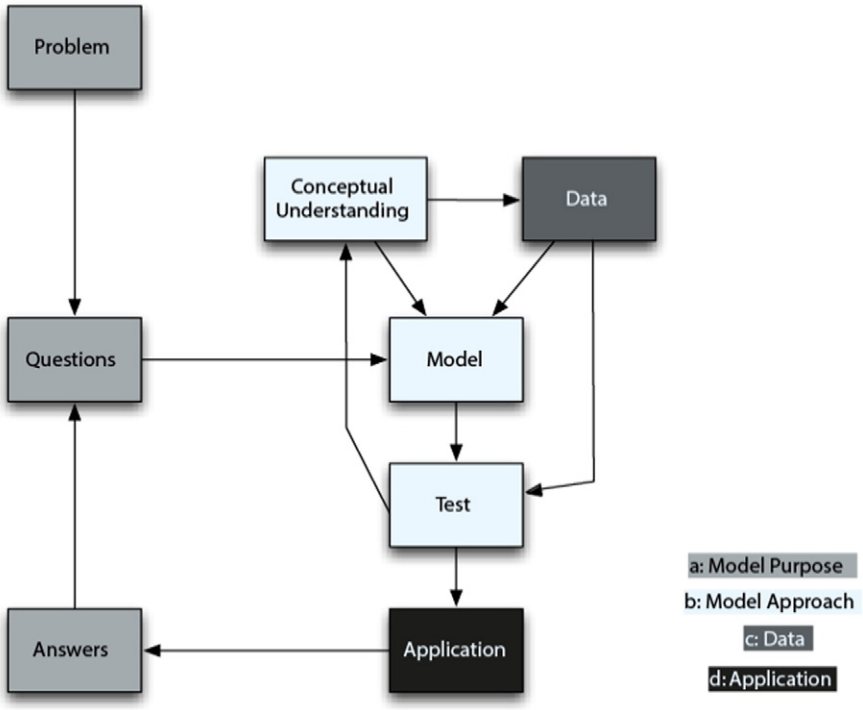


Fig. 1. Generic iterative modelling process used to generate answers (and new questions) to environmental problems.

(Kay et al., 2010). Such predictions are complicated by the effects of scale, such as its impact on lag times between management actions and observed water quality improvements (Murphy et al., 2015a). In addition, calibrating FIO model simulations of mitigation effectiveness can be hampered by a lack of good quality FIO data (e.g. losses and exports) at the farm scale (Muirhead, 2015; Coffey et al., 2010, 2013). While generic management actions can be incorporated into models at a coarse resolution (e.g. typical manure application periods and grazing durations) it is the subtleties of management actions that are notoriously difficult to capture in model frameworks. This difficulty is largely because management is not static over time and changes in management at the farm business level can lead to discrepancies between on-the-ground actions versus modelled assumptions (e.g. grazing regimes and manure management) (Winter et al., 2011). Model frameworks need flexibility to respond to shifts in management practice (e.g. Bloodworth et al., 2015); the development of novel modelling approaches are now urgently required to better represent the effects of changing management actions on FIO dynamics.

2.2. Modelling approach: what approach should be used and why?

The structure of a model is based on the conceptual understanding of the system of interest. Conceptually, the framing of how microbial fate and transfer interact in agricultural systems is improving but the conversion of perceptual and conceptual understanding into procedural models is fraught with challenges (Krueger et al., 2007). One significant barrier is the level of uncertainty in answers to fundamental research questions (Section 1). In the UK and Europe, this is largely due to a legacy of riverine monitoring programmes that have historically focussed on nutrient rather than microbial pollutants, leading to relative scarcity of spatially distributed FIO data in catchment systems (Kay et al., 2007). This is coupled with a greater focus on longer-term monitoring of bathing waters (end-point receptors) as driven by the BWD and risks from sea-bathing. In contrast, countries like New Zealand, the USA and Canada carry out much greater spatial sampling of microbial water quality across catchments, driven by cultural differences in recreational pursuits and interactions with waterbodies e.g. differences in river versus sea-bathing, and therefore arguably have a far better spatial understanding of catchment microbial dynamics relative to the UK (Wilkinson et al., 2011). The amenity value of surface water bodies and coastal waters therefore plays a significant role in governing the availability of existing large-scale FIO datasets.

Whatever level of underpinning knowledge, there are a number of different modelling approaches available for exploring FIO dynamics in catchment systems in response to the purposes outlined in Section 2.1. These can include export coefficient and regression (McGrane et al., 2014; Sinclair et al., 2009; Kay et al., 2008b; Crowther et al., 2002), probabilistic or risk based approaches which represent inputs or parameters as probability distributions, that can be propagated though the model analytically or numerically (e.g. using Monte Carlo simulation) (Muirhead et al., 2011) and mechanistic/process-based models (Iudicello and Chin, 2015; Coffey et al., 2010; Ferguson et al., 2007). These approaches operate at different temporal resolutions, or time-steps, ranging from sub-daily through to annual or longer timeframes and, as with spatial scale, the temporal scale of operation should help to dictate the best approach for the question of interest. In addition, the transferability of these different approaches across contrasting agricultural systems needs attention, with a particular focus on the challenges posed by inherent differences in catchment characteristics.

The real-time prediction of water quality at bathing areas is a topical modelling challenge in the UK. It has received increased impetus following revisions to the BWD that allow for discounting of a proportion of regulatory samples of poor microbial water quality if information has been provided to the public to warn about a risk of exposure to substandard water quality (e.g. via real-time electronic signage systems). Targeted monitoring has revealed that FIO concentrations exhibit diurnal variability on any given bathing day and that the variation can span across different bathing water classifications (Wyer et al., 2013). This diurnal variability provides clear rationale for the need of models that can dynamically account for FIO behaviour at a sub-daily time-step for informing improved real-time predictions. In Scotland the forecasting of bathing water quality is built around a simple decision-tree approach utilising river discharge and antecedent rainfall information (Stidson et al., 2012). In the USA the software package 'Virtual Beach' develops site-specific statistical models (including multiple linear regression) for the prediction of FIOs at recreational beaches (Frick et al., 2008). For wide-scale adoption these predictive tools need to be developed for each individual bathing site and cannot necessarily be directly transferred to another bathing site without modification.

More sophisticated models, with inherent complexity in the model structure, may not (yet) deliver useful results for such purposes. Complex models often require considerable expertise and resources for computations, data preprocessing, or data post-processing. As a result they are poorly suited to operational applications that require real-time data processing. In addition, users of complex environmental models often fail to deal with uncertainty in their predictions due to the computational expense; however, when they do provide uncertainty estimates these are often ignored or misused by decision-makers (Beven, 2009). Sometimes, a simple model approach can be more effective in guiding decisions or informing knowledge than a model that attempts to capture a comprehensive range of catchment processes and interactions. Simple models also accommodate uncertainty but often users of these approaches have a greater trust in outputs because of increased transparency of the inner workings of the tool.

In moving from a more complex to relatively simple approach it is likely that the original question we are asking of the model needs to be reframed in order to accommodate a different modelling strategy. One simple approach is to develop a risk index where the aim is to provide an indication of the relative contribution of different sources of faecal contamination to the aquatic environment (Muirhead, 2015; Oliver et al., 2010). These models can take into account many of the underlying processes of source, mobilisation, transport and connectivity to streams but do not explicitly model the processes, and often incorporate expert judgements to inform the risk index (see Fish et al., 2009). This approach can indicate the expected relative change in stream FIO concentration and identify the largest FIO sources, which is useful for prioritising mitigation programs, but generally does not attempt to predict in-stream FIO concentrations (Muirhead, 2015). Advantages of the risk index approach are transferability (providing the sources are consistent) and the ability to easily modify the calculations used as new information/knowledge becomes available.

In a recent review, de Brauwere et al. (2014) commented that regression-based models cannot *replace* mechanistic models for long term assessments of management practices or understanding underlying FIO dynamics. Regression models are not constructed for this purpose thus their application in this context would reflect a case of model misuse. Replacing one model with another is not always necessary or desirable but recognising their different underlying purposes is clearly important. There is even much to be gained from observations of model failure in a particular context. Utilising models is a learning process, valuable insight can be gained from examining why a model fails to match observations, which can in turn lead to the formation of new hypotheses and novel questions. Part of this learning process should ensure that sensitivity and uncertainty analysis is embedded within the modelling approach (Beven, 2015), although to date relatively little attention has been given to these aspects of FIO modelling.

Approaches to modelling can also be strongly shaped by co-operation. There are inefficiencies associated with model proliferation, where multiple groups working on a particular topic develop their own model. Reducing duplication of effort is important if advances in FIO modelling are to be optimised. The need to purchase software

licences or the lack of access to source code can prevent other researchers from exploring the power, transferability and potential of different models for their respective FIO datasets. The promotion of collaboration, transparency and open source code would open up model architecture to new ideas from different FIO model developers and accelerate improvements, opportunities for transferability, or new applications of existing model frameworks (Wilkinson et al., 2015). In doing so it is paramount to stress the need for version tracking and quality control protocols in order to capture the reporting of model modifications and data provenance (Vitolo et al., 2015). Without doing so there is an increased risk of models being developed without full audit trails of how they have evolved and without the associated narrative of why they are performing in such a way. The development of FIO models without tracking such changes could negate the benefits of opening up source code to the developer community given the pace at which people (and expertise) move on institutionally. Recent developments in software publishing now allows for model developers to gain recognition for publishing models and source code in the public domain. However, there is a need to support developers to maintain and develop the approaches once funded research projects have been completed.

2.3. Data availability: what data do we need and what is available?

Often our ability to model pollutant response and behaviour in the environment runs ahead of the data that is available to drive or test such models. This is not an issue that is unique to microbial pollution in catchment systems. There is, however, a *relative* lack of data for FIOs when compared with other pollutants monitored in agricultural catchments (Muirhead, 2015). This is partly a legacy of a focus on nutrients in catchment monitoring, together with generally poor central data management of academic, agency and private data resources. Furthermore, monitoring data is designed to determine water quality at a given location, rather than understanding where the contaminants are coming from and therefore, often lacks data at key times and/or locations needed to calibrate models (Wilkinson et al., 2011).

Beyond the immediate issues of spatial and temporal quality of historical datasets and associated sampling capability, there still exist a number of gaps in fundamental understanding of FIO processes in the environment. Progress is being made but issues remain, for example, in determining good quantitative data on wildlife contributions to FIO loading in, and export from, agricultural catchments (Coffey et al., 2015; Guber et al., 2015), securing a robust library of FIO die-off in fresh faeces of younger livestock (Oliver et al., 2012a), obtaining robust parameters to enable prediction of manure release and removal in site-specific conditions (Blaustein et al., 2015a, 2015b, 2016), incorporating bed sediment reservoirs of FIOs into existing modelling frameworks (Coffey et al., 2014) and also in understanding the contributions of septic tanks to the impairment of microbial water quality. Septic tank inputs of P to watercourses are now gaining significant attention (Withers et al., 2014) and in many ways this has accelerated the focus of their potential role on FIO contributions to the aquatic environment — helping to 'bridge the gap' between these two aspects of diffuse pollution research. This represents an idea (based on anecdotal association) linking nutrient to FIO research that has had a positive impact. However, it has progressed because of the testing of hypothesised links so that the cross pollination across research disciplines contributed inspiration rather than allowing anecdote to prevail over evidence.

Techniques such as flowpath separation are also attracting recognition in terms of their value for advancing our understanding of FIO transfer dynamics in catchments (Murphy et al., 2015b). However, there remain significant issues with currently available data, and in particular the rates of persistence of FIOs within the multitude of different environmental matrices that they are associated with, e.g. freshwaters of varying turbidity, different soil classifications, and there remain limited field-relevant studies relative to laboratory-based reporting of FIO population dynamics in environmental matrices. Contributions of FIOs from groundwater sources also reflect a relatively unexplored area in the field of catchment microbial dynamics. Certainly the majority of FIO models typically do not consider groundwater contributions as a source of faecal pollution or more specifically the distribution of inputs from groundwater as a source of low FIO input to surface waters via baseflow. Data needs, such as those described above, are fundamental for the advance of FIO modelling and prediction, and the parameterisation of models of FIO behaviour. There needs to be an increased effort to evaluate ranges of FIO parameters during the model parameterisation process; making datasets more transparent and more widely available will help facilitate this.

With data that are available there will remain questions over their transferability to different environmental contexts. Many of these questions could be addressed by providing more detailed meta-data (e.g. weather variables and catchment characteristics) associated with the experimental conditions or monitoring programmes that have generated the data. While the research community may want 'everything' in terms of accompanying data, in reality there are obviously cost and resource constraints that limit wider data collection. Opinions differ on what environmental data should be provided to support FIO modelling, highlighting the need for the research community to debate and identify a 'baseline' of essential supplementary information to facilitate international transferability of FIO data. One basic example is the coupling of FIO concentration and discharge data in hydrological studies; concentration data alone inhibits a wider assessment of catchment issues and exported FIO loads (Pachepsky et al., 2006).This opens up wider debates as to whether arithmetic or geometric mean FIO data should be combined with discharge, and how to compare FIO concentrations determined by different methods (e.g. membrane filtration versus most probable number).

In some countries, nationally available datasets or data derived from farm and fertiliser practice surveys can be explored in further detail to try to redress some of the finer-scale issues of management impacts on FIO dynamics (e.g. Aitken, 2003). Key data that can be extracted from such sources for onward use in FIO modelling include: information on yard management (clean and dirty water separation); frequency of livestock stream fording; and manure management including computed ages of manures and slurries at time of application to land. Access to, and knowledge of, such sources of supplementary data can be enhanced by the involvement of stakeholders and anticipated end-users throughout the entire modelling process, from development to evaluation (Hamilton et al., 2015). Further research is needed to enable successful and reliable integration of mitigation and best management practices (BMPs) into model space but there are large collections of supplementary data that can be explored in order to strengthen FIO modelling for some purposes. However, it is likely that FIO source apportionment or model calibration can be especially sensitive to biased assumptions about practices (e.g. cattle access to streams and duration of manure storage) in particular catchments, based on the downscaling of regional or national surveys of farm practices. Therefore improvements in farm activity data collection will always be welcome to better inform FIO modelling.

2.4. Model application: how do we apply our model (effectively)?

Applying and testing models in landscapes typical of different catchment systems around the world enables an assessment of how transferable a model structure might be beyond its calibration catchment in order to evaluate its global applicability. Transferability of model structure is a favourable attribute but one that presents considerable challenges at the international level, largely as a result of availability of the datasets used to drive models, subtle differences in the classifications used within such datasets across different nations, and given that different people are all asking subtly different questions. Source loads (species, prevalence, concentration etc.), FIO die-off, FIO-sediment interactions and other fate/transport parameters are non-transferable

in an environmental context. Values selected are often used as a means of model calibration without any empirical or physical justification. The model parameterisation process needs to be coupled with wider discussion and inclusion of statistical methods (e.g. probabilistic treatment and propagation of parameter uncertainty) to improve model design. This treatment would help to account for specificity of FIO data in model performance evaluation and model calibration.

Awareness and respect for different modelling approaches is also important. Those that apply process-based FIO models (e.g. SWAT and HSPF) generally argue that despite their limitations there is no viable alternative (Pachepsky et al., 2006). However, with questions increasingly focusing on when and where to prioritise spatial targeting of mitigation and management within catchments there is an emerging need for models that take a risk-based approach (e.g. Reaney et al., 2011; Oliver et al., 2010), which highlight in relative (rather than absolute) terms, areas of catchments most conducive for facilitating FIO transfer from land to water. Export coefficient models can do this too but a risk-based approach is the simplest approach to take and prioritisation does not need anything more complex. Something as simple as a risk based model is therefore consistent with the level of uncertainty in the data that underpins it. Although these types of models have not yet been widely adapted for modelling FIOs, risk-based approaches could be parameterised with existing datasets, which is in contrast to the current overreliance on deterministic complex models that often lack the availability of data needed to drive those models effectively (Dean et al., 2009). The selection of useful models for inappropriate applications therefore needs to be more thoroughly guarded against by both the user and developer communities. Legacy effects of 'go-to' industry-standard models being used over long time-periods may be one reason for a mismatch of model application relative to purpose. These 'work-horse' models may be deployed to tackle new and emerging questions that they were simply not designed to answer even with modification or integration of new FIO modelling routines.

Finally, important advances in the science of catchment microbial dynamics often remain inaccessible to those who manage landscape risk on a day-to-day basis. The extent to which models are useful, and that they are used, is driven not only by the rigour of the model but also by the needs of the user, and the availability and accessibility of the model. There are important technical questions around the usability and visualisation of models, and this remains an area of active research (Karpouzoglou et al., 2016; Rink et al., 2014). Visualisations of environmental risk can powerfully communicate complex environmental risk assessments to decision-makers (Lahr and Kooistra, 2010). Yet many attempts at risk communication are poorly received by end-users (Oliver et al., 2012b), largely because they fail to engage and involve their target audience in the design of such tools (Whitman et al., 2015). Thus, where models or their visualised outputs are intended as tools to help people understand risk, a 'human-centric' approach is required. Studies vary in the point at which model developers seek participation from those that might use the model e.g. from interpretation and modification of visualisation, through model development to definition of the initial research question. These participatory approaches can force model developers to alter both their focus and their ways of working. This shift can be uncomfortable and though calls for participatory modelling are common, examples of its application are far rarer (e.g. Landstrom et al., 2011; Whitman et al., 2015).

3. Horizon scanning & future opportunities

Challenges for the future of FIO modelling in agricultural catchments include, but are not limited to, the need for good quality data on FIO fate and behaviour in the environment. Here we build on the issues identified through our discussion of the four over-arching questions associated with good modelling practice and map future research priorities in terms of short (<5 year) and longer-term (5-10 year) needs (Table 1). As these priorities are addressed, a pathway to more effective deployment of models for characterising catchment microbial dynamics should begin to emerge.

3.1. Short term research needs (0–5 years)

Modelling of microbial pollutants in agricultural catchments is only as good as the data that drives the model. Review articles and commentaries often feature repeated pleas for research to 'plug the gaps' in understanding that may begin to sound overused, but for FIO modelling those gaps are surprisingly large (and more so for specific pathogens) and seriously compromise modelling efforts to deliver wider environmental benefits. A case in point is the lack of relevant data concerning wildlife contributions to catchment FIO dynamics. The lack of data on wildlife/wildfowl FIO sources and their potential importance were reported in the literature almost 20 years ago (Weiskel et al., 1996), and while some effort is now being converted into published findings (Guber et al., 2015; Muirhead et al., 2011; Kiefer et al., 2012), international coverage of useful information remains weak. Uncertainty in FIO loading from wildlife and wildfowl, and behaviour of these FIO populations can increase the uncertainty and undermine model predictions of microbial pollution in agricultural systems. Where FIOs are apportioned to livestock, the agricultural sector will often respond by querying the relative contribution of migratory wildlife or wildfowl. This issue is further exacerbated by the difficulty in calculating faecal loadings since this requires the weight of faeces, its microbial concentration and correct algorithms to calculate the true FIO loads (Muirhead and Cave, 2014). Without being able to understand and evidence these contributions, scepticism over model outputs among some catchment stakeholders will remain high. In parallel, and to help facilitate fundamental data collection such as that described above, a co-ordinated clear voice is needed from the international FIO research community to highlight the relative scarcity of empirical data, and established meta-data standards, across a broad spectrum of environmental conditions.

The pursuit of good quality FIO data does need to be complemented with continued efforts to understand the differential behaviour of FIOs and pathogens, and the associated implications for modelling the efficacy of mitigations designed to reduce microbial watercourse pollution. Thus, while we have focussed our discussion on FIO modelling it is important for resource managers and policy makers to recognise that FIO models do not necessarily inform on specific pathogen behaviour. However, the nexus of FIO modelling and risk assessment is gaining

Table 1
Summary of future short- and longer-term research opportunities for faecal indicator organism (FIO) modelling.

Future research opportunities for FIO modelling	Time-frame
Improve the underpinning evidence-base of FIO fate & behaviour in the environment	<5 years
Strengthen the available data on wildlife/wildfowl FIO sources	<5 years
Increased consideration of the role of groundwater contributions as a source of faecal pollution	<5 years
Better understanding of the differential behaviour of FIOs & specific pathogens	<5 years
Future FIO model performance criteria to include, as a minimum, an uncertainty analysis of modelled predictions	<5 years
Identify a 'baseline' of essential supplementary information to facilitate international transferability of FIO data	<5years
The integration of dynamic management practices and mitigation options into FIO model space within a wider framework of climate and land use change	<10years
Extrapolating FIO fate & transport data from experimental plots to fields and catchments (scaling methodologies)	<10 years
Innovative combinations of FIO modelling and MST for informing on catchment microbial risks	<10 years
Integration of different modelling approaches (including risk-based approaches & QMRA) to promote more holistic modelling of catchment microbial dynamics	<10 years

MST: Microbial Source Tracking; QMRA: Quantitative Microbial Risk Assessment.

significant momentum and the use of quantitative microbial risk assessment (QMRA) offers another modelling framework with which to estimate human infection risk from exposure to pathogen contaminated waters (Soller et al., 2015).

Benefits of FIO modelling will be further enhanced if the research community promotes a consistent message to model developers calling for any future model performance criteria to include, as a minimum, an uncertainty analysis of modelled predictions. Thus, the pedigree of uncertainty associated with model outputs needs to be transparent and included as standard in the reporting of any FIO modelling. There are mechanisms that can help deliver this drive for greater awareness of model uncertainty. For example, there are more frequent opportunities to promote knowledge exchange (KE) across the science-policy interface enabling scientists and policy-makers to debate the role and impact of model uncertainty. Research Councils in the UK, and in other nations too, are increasingly funding policy-placement opportunities whereby scientists are embedded within government departments thus providing an important route for aiding KE. This should be encouraged in the general field of environmental decision-making using models. In addition, those responsible for funding research could improve model transparency by ensuring that projects with a modelling component fulfil basic uncertainty analysis criteria. Indeed, several academic journals, whose remit includes environmental modelling, now stipulate uncertainty analysis of any modelling as a prerequisite for publication. This template should also be adopted at the funding stage for research projects.

3.2. Longer term research needs (5–10 years)

Increased mutual respect for different modelling philosophies, including those that deviate from a process-based approach (e.g. Odoni and Lane, 2010) and also in promoting a more co-ordinated strategy for the integration of different disciplinary expertise is essential (Hamilton et al., 2015). Convincing model developers that sometimes their own model is not the right tool for the job can be a problem across environmental modelling (Prell et al., 2007). Arguably the biggest risk to modelling frameworks is a shift in the conceptualisation of how the system operates. From an environmental perspective this is perhaps not likely, but the management of agricultural systems is more dynamic and able to accommodate change. Thus, there is a need to ensure that modelling efforts are able to reflect those changes should they occur — this equates to flexibility and futureproofing of modelling approaches and anticipating dynamic agricultural practices within a wider framework of climate and land use change (Coffey et al., 2014). Such efforts are attractive but extremely difficult in practice given the multitude of different changes that must be accounted for. Less flexible modelling approaches will be more at risk of becoming outdated — this is not necessarily a problem if outdated models are recognised rather than continually supported as a legacy of end-user preference. The integration of dynamic management practices and mitigation options into FIO model space represents a clear challenge for model developers. While there is undoubted progress on this challenge it is hindered by the gaps in empirical data and understanding described above.

Efforts to future-proof modelling approaches must equate to an increased effort by the research community to focus on the development of scaling rules for FIO behaviour to enable greater confidence in extrapolation of findings from smaller to larger scales. Extrapolating FIO fate and transport data from experimental plots to fields and catchments will require accounting for increased opportunities for in-field FIO intermittent accumulation, growth and inactivation, spatial variability in overland flow discharge and frequency, etc. Experiments to understand this scaling are difficult and costly, but necessary to increase the value of plot studies. The use of FIO modelling to support the emerging science of microbial source tracking (MST) will also serve to strengthen the toolbox of techniques available to environmental managers for assessing microbial risks in catchment systems. Though MST remains largely qualitative and the subject of much debate with regard to source sensitivity and source specificity (Astrom et al., 2015) it is a technique that is gathering pace and innovative combinations of FIO modelling and MST may hold promise for informing on catchment microbial risks in the future. Likewise, more real-time monitoring techniques are being explored and utilised by researchers to understand temporal variability in faecal contamination of transient surface and groundwater systems (e.g. Sorensen et al., 2015). This presents both an opportunity and a challenge for improved modelling of FIO transfers in the environment.

Given the difficulties of FIO and pathogen data collection in catchments, modelling could be deployed to help guide monitoring programs. Currently, questions of when, where and how to sample are not driven by FIO model calibration, sensitivity analysis, uncertainty evaluation, data assimilation, or other operations that improve modelling reliability and usefulness. For example, storm-flow can export up to 98% of the annual *E. coli* load from agricultural catchments but represent only 6–30% of routine water quality monitoring samples (Muirhead, 2015; McKergow and Davies-Colley, 2010). Longer term challenges should reflect a move to more integrated approaches to modelling. To realise this ambition requires an appreciation from the regulatory and policy communities that different types of models can be applied in unison to complement rather than 'replace' each other addressing different parts of the larger, multi-scaled problem of integrated catchment management. Integrating different modelling approaches to promote a more holistic approach to catchment modelling is challenging. The development of engaging user interfaces, the incentivising of 'opening-up' the underlying model source code and enabling wider access to multiple model platforms free of licencing issues will require co-operation and collaboration across multiple disciplinary fields and a range of organisations. Most notably, links across psychology, the social and environmental sciences and the environmental modelling community need to be strengthened even further to ensure better human-computer interactive experiences in the modelling process.

4. Conclusion

Modelling microbial fate and transport has been, and will continue to be, helpful in elucidating and integrating knowledge about the intimate relationships between water, soil, FIOs and catchment management. Thus, modelling of catchment microbial dynamics supports our efforts to bridge scales between research and policy making, and plays an important role in helping to understand and address the challenges of protecting food safety and water quality in the face of climate and land use change. Current environmental agendas and increased awareness has put FIO research in focus for many national and international bodies and groups meaning that the time is now right to revisit, revise, and advance factual, conceptual, and technical foundations of FIO fate and transport modelling. Using the recommendations from the overarching questions posed in this commentary will help to promote better model deployment in the field of catchment microbial dynamics.

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Predicting microbial water quality with models: Over-arching questions for managing risk in agricultural catchments

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