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Development of a Decision-Support Tool for Identifying the most Suitable Approach to Achieve Nitrate Source Determination

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SCHOLARONE[™] Manuscripts At the moment, the field of nitrate source determination is fragmented and approach dependent. This makes it challenging for stakeholders to identify the most suitable approach and analytical technique to use in the event of a pollution incident involving nitrates in water. To address this gap, this paper examines the development and application of a decision-support tool to support environmental forensics studies for nitrate contamination. In particular, this tool can support policy makers, regulators and operators within the field in understanding the environmental hazards and processes resulting from nitrate contamination, and to implement appropriate actions for limiting the impacts that may arise from such contamination.

Graphical Abstract

Numerous approaches have been suggested for differentiating point and diffuse sources of nitrate contamination, including stable nitrate isotopes, microbiological analyses, genetic markers and chemical markers. Each approach has its own strengths and limitations. As a result, the most appropriate approach to use largely depends upon the scenario and the context of the study. However, available data on nitrate source determination is highly fragmented and approach dependent, with very little if any interface between the different techniques. This makes it difficult for stakeholders to identify the most suitable approach to adopt in a specific scenario. Therefore, this paper examines the development and application of a decision-support tool to support environmental forensics studies for nitrate contamination. In particular, this tool can support policy makers, regulators and operators within the field in understanding the environmental hazards and processes resulting from nitrate contamination, and to implement appropriate actions for limiting the impacts that may arise from such contamination. The tool was developed using the IDEF0 modeling system, and evaluated by interviewing key

1. Determine Scenario Context Scenario Characteristics Differentiation Objectives Evaluation Criteria Site racteristic: Scope Criteria Lis veed for NSD Potential Sources 2. Determine Differentiation Criteria Required Differentiation Available Resources Differentiati Level Budge Deadline Expertise Available Funding Factor Importance Priority Lis 3. Determine Differentiation Approach ach Criteria Appro Approau. Criteria Comparative Analysis Confirm scope has been met Identify Potential Approach Potential Validate Choice

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Development of a Decision-Support Tool for Identifying the most Suitable Approach to Achieve Nitrate Source Determination

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Numerous approaches have been suggested for differentiating point and diffuse sources of nitrate contamination, including nitrate stable isotopes, microbiological analyses, genetic markers and chemical markers. Each approach has its own strengths and limitations. As a result, the most appropriate approach to use largely depends upon the scenario and the context of the study. However, available data on nitrate source determination is highly fragmented and approach dependent, with very little if any interface between the different techniques. This makes it difficult for stakeholders to identify the most suitable approach to adopt in a specific scenario. Therefore, this paper examines the development and application of a decision-support tool to support environmental forensics studies for nitrate contamination. In particular, this tool can support policy makers, regulators and operators within the field in understanding the environmental hazards and processes resulting from nitrate contamination, and to implement appropriate actions for limiting the impacts that may arise from such contamination. The tool was developed using the IDEF0 modeling system, and evaluated by interviewing key stakeholders who suggested a number of important implications for practice.

Introduction

Today, the nitrate ion is considered to be an environmental contaminant of concern because the existence of various point and diffuse sources has made it a ubiquitous contaminant of natural water resources. In addition its presence within water bodies has been linked to various environmental and health effects. In order to achieve improved water resource management and preserve water quality, it is imperative that the sources of nitrate contamination can be identified. This allows for more efficient remediation efforts and more effective application of the 'polluter pays principle'.

To date, numerous approaches have been suggested for differentiating point and diffuse sources of nitrate contamination within water bodies. These include the use of nitrate stable isotopes,^{1,2} microbiological analyses,³ genetic markers,⁴ and chemical markers.¹ These approaches each have their own strengths and limitations in determining the sources, movement and distribution of the various point and diffuse sources of nitrate contamination. As a result, the most appropriate approach to use largely depends upon the specific scenario and the context of the study. However, available data on nitrate source determination is highly fragmented and approach dependent, with very little or no interface between the different techniques. This makes it difficult for stakeholders to identify the most suitable approach to adopt in a specific scenario. Aggregating the present knowledge into a unified system makes it easier for stakeholders to assess and implement

the most appropriate approach for their specific scenario. Therefore, a decision-support tool was developed using the Integration Definition Function (IDEF0) modeling system.⁵ The developed tool's aim is to provide a generic framework that formalizes the thought processes that need to be carried out in order to identify the most suitable approach to adopt for achieving nitrate source determination in a specific scenario. Hence, through the tool's application, the approach selection is more easily justified and the outcome of studies related to nitrate source determination are standardized.

Through the inclusion of supplementary material, which brings together the current state of knowledge in the area of determination and the differentiation nitrate source requirements of key stakeholders, the selection of the most appropriate approach is facilitated. In addition to the afforded by each differentiation potential approach, considerations such as cost, time, sample volumes and the state of the approach are taken into account. Hence, this tool optimizes the effectiveness of environmental forensics studies for nitrate source determination by assisting in the process of ensuring that the most suitable approach is applied within a specific scenario.

Therefore, this paper examines the development and application of a decision-support tool to support environmental forensics studies for nitrate contamination. In particular, this will support policy makers, regulators and operators within the field in understanding the environmental hazards and processes resulting from nitrate contamination, and to implement appropriate actions for limiting the impacts that may arise from such contamination.

Method

System Selection

A number of multi-criteria decision analysis systems can be used in the development of decision tools. These are largely functional modeling methods, where activities, actions, processes and/or operations, collectively known as functions, are represented in a systematic manner. Within this study, the IDEF0 modeling system was adopted for the development of a decision tool for nitrate source determination. This is a public domain modeling system that outlines the way a model is developed and depicted.⁵ To date, IDEF0 has been used to model a number of systems, such as the development of hospital waste management programs and emergency management procedures.^{6,7} By depicting and formalizing the thought processes that need to be carried out, bottle-necks and/or deficiencies within the methodology can be more easily identified.

An IDEF0 model consists of a hierarchical series of IDEF0 diagrams, which consist of a series of boxes and arrows (Figure 1). Boxes depict the functions that need to be fulfilled, whilst the arrows represent the functional relationships, which may be inputs (I), controls (C), outputs (O) and mechanisms (M). These are collectively known as ICOM arrows. The presence of a node ID identifies further sub-divisions within a child-diagram.



Figure 1: IDEF0 basic components

The strengths of the IDEF0 modeling system include that it is generic, rigorous and precise, concise, conceptual and flexible.5 This is because it allows for a consistent representation of the various functions (activities, actions, processes and/or operations that need to be fulfilled) and functional relationships (the way the various functions interlink together as inputs, controls, outputs and mechanisms) that are necessary for the overall model aim to be achieved.⁵ This makes IDEF0 particularly relevant for developing decision support tools such as the subject of this paper. IDEF0 allows for correct and usable models to be produced, which may be successfully applied to scenarios with varying purposes, scopes and complexities. The reason for this is that IDEF0 focusses on the identification of functional requirements as opposed to physical or organizational requirements. At the same time, the developed model is concise, thereby facilitating the modeled system's communication and validation. These are essential

considerations in environmental studies, where the organizations carrying out the investigation have varying requirements, scopes and resources, yet comparable outcomes are necessary in order to achieve effective source determination as the first step in implementing remediation actions.

Decision Tool Development

Decision tool development was carried out according to the methods specified by the Federal Information Processing Standard (FIPS) 183 for IDEF0 modeling,⁵ which is maintained by the National Institute of Standards and Technology (NIST). In summary, the method consists of the initial identification of the model's context, viewpoint and purpose, which is also known as the model's orientation, and is depicted within the top-level A-0 context diagram. The high-level function that is outlined in the A-0 context diagram is then decomposed into the main sub-functions, which results in a hierarchical series of diagrams. Any supporting materials are also developed.

Model Evaluation

Model evaluation was carried out in a two-step process of model verification followed by model validation. Model verification involves ensuring that the model was correctly developed, thereby allowing for the required specifications to be achieved. Meanwhile, model validation ensures that the developed decision tool carries out its intended function and that it meets the requirements of its users

Results and Discussion

Decision Tool Development

The developed model consists of a 3-level hierarchical model, which was considered to be a suitable definition of the decision-processes required for identifying the most suitable technique for differentiating between sources of nitrate contamination. The top-level context diagram, A-0 (Figure 2), identifies that the overall model consists of one input (I1), one output (O1), four controls (C1, C2, C3, C4) and one mechanism (M1). Since the approach to be taken (O1) largely depends on the scenario under study (I1), these have been identified as the model's only overall output and input, respectively. However, additional interim outputs do emerge throughout the course of the model's application.

A number of controls were identified to constrain the transformation of the scenario (the input) into the identified approach (the output). The relevant legislation under which this study is operating is the first control (C1). The legislative control depends on the particular scenario. It is likely to be the Environmental Liability Directive (or equivalent outside of Europe) and additional legislation such as the Nitrates Directive and relevant case law. The specific requirements (C2) of the entity carrying out the study are a second control mechanism. They determine the scope of the study and the extent to which the sources of nitrate contamination are differentiated and, therefore, the approach to be taken. The third control mechanism is that of available resources (C3), which considers such factors as time and budgetary restrictions, as well as the level of expertise available. The final control mechanism represents the characteristics of the various approaches (C4) that determine the outcome of the model's implementation.

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Figure 2: The top-level A-0 context diagram.

The functions within this model are carried out by the project team that is identifying the most suitable approach to differentiate the sources of nitrate contamination under the guidance of the environmental officer. Therefore, the project team represents the model's only mechanism (M1). The project team would be headed by the environmental officer from whose viewpoint this model is developed (Figure 2). However, this individual would require inputs from relevant individuals within and external to the organization, as necessary, such as financial officers, legal experts and scientific personnel.

On the basis of the model's context given in the A-0 diagram, further functional decomposition was carried out, thereby representing the process of transforming the model's overall input (I1) into an output (O1) in greater detail. The full model decomposition is presented in Figures 3 and within the Supplementary Material (Figures S.1 – S.3). In summary, the top-most diagram (A0) is the only child-diagram of the A-0 top-level context diagram, where the model's global function defined within the A-0 diagram is sub-divided into the third tier of functionality, which consists of three functions:

- 1. Determine the context of the scenario in which this model is to operate (Function 1): Why is differentiation needed? A1 diagram.
- 2. Determine the differentiation criteria of interest within the specific scenario (Function 2): What should differentiation achieve? A2 diagram.
- 3. Determine the differentiation approach (Function 3): How is differentiation going to be achieved? A3 diagram.

Each function within the A0 diagram is, then, further decomposed into a corresponding child-diagram. Within the model presented here, no additional child-diagrams arising from this third tier were necessary, because the model was considered by the authors to be sufficiently detailed at this stage to achieve the requirements of a nitrate source determination study.

In order to facilitate the model's application by individuals who are not familiar with the IDEF0 methodology, a summary was developed to complement the IDEF0 model based on the developed IDEF0 model described, which ensures the model's robustness. Two complementary summaries were prepared, one in the form of a flow chart (Figure) and another as an accompanying table of questions (Figure 5)

Figure 3: The A0 diagram: Process of Approach Identification

Supporting Material

As previously mentioned, a limitation of currently available data on nitrate source determination is that it is highly fragmented and approach dependent. This factor makes it very difficult for stakeholders to identify the most suitable approach for a specific scenario, unless suitable resources and expertise is available for a comprehensive review of literature. Since the users of this model are expected to be individuals within policy development, regulatory bodies and operators it is unlikely that such resources are available within the organization itself.

Since IDEF0 models are largely conceptual, the developed model is not suitable for resolving issues related to the fragmented nature of the current state of knowledge. This role is fulfilled through the addition of supporting material to complement the decision framework illustrated within the IDEF0 model. This supporting material, therefore, makes the developed decision tool easier to implement in the developing of nitrate source determination studies.

Of note is that an advantage resulting from the nature of the IDEF0 modeling system is that the decision tool developed would not require frequent updating. Rather, it is this supporting material that needs to be updated on the basis of new advances in the number and variability of approaches that are developing in this evolving field. This factor facilitates the application of the developed decision tool as it eliminates the need for an overhaul of the entire tool on a regular basis.

The availability of supporting material was identified to be particularly critical in relation to the model's fourth control (C4: Approaches). Data related to controls C1, C2 and C3 (legislation, requirements and available resources) are largely scenario dependent. Therefore, they need to be identified by the organization carrying out the analysis. However, the potential pool of approaches is universal. The developed supporting tables, therefore, allows for the four main approaches that have been largely adopted for nitrate source determination (nitrate isotopes, genetic markers, microbiological analyses and chemical markers) to be compared.



Figure 4: Decision tool summary flow chart.

A0 Identify Approach to Differentiate Nitrate Sources of Contamination

The first supporting material prepared outlines the level of differentiation that the various approaches can achieve (Table 1). From Table 1, it can be seen that consecutive sources of contamination in a column with the same shade cannot be differentiated using that particular approach. For example, nitrate isotopes cannot differentiate between different sources of manure and sewage (both in group 1 for nitrate isotopes), but can differentiate between fertilizer nitrate (group 3) and soil nitrogen (group 4) and ammonium in fertilizer (group 6). Chemical markers, then, can differentiate between three classes (manure, raw and treated sewage) but cannot differentiate between different sources of manure (eg cattle or sheep). Whilst all four approaches may identify the presence of fecal contamination (manure and sewage), only nitrate isotopes can identify inorganic nitrogen fertilizer. Similarly, only chemical markers are able to differentiate between raw and treated sewage. Finally, as genetic markers are host specific, they may differentiate between different sources of manure but they are unable to differentiate between raw and treated sewage.

A1 Determine Scenario Context	Why is differentiation needed?
	What are the site characteristics?
	e.g. What is the composition of the catchment?
11 Identify Scenario Characteristics	What is the expected temporal and spatial variability?
	Why is nitrate source determination required?
	What are the potential sources?
	What are the study's objectives?
12 Determine Differentiation Objectives	e.g. Is it a scoping study or is it for legal action?
	What are the factors of interest in this study?
13 Determine Evaluation Criteria	e.g. Operationally, do cost, time, expertise and/or robustness have decisive roles?
A2 Determine Differentiation Criteria	What should differentiation achieve?
	What level of differentiation is required?
21 Identify Level of Differentiation Required	e.g. Is presence-absence of a particular source or source attribution required?
21 Identity Level of Differentiation Required	Do the various inorganic or organic sources need to be further differentiated?
	Is differentiation based on entry route (e.g. raw and treated sewage) required?
	What budgets are available for this study?
22 Identify Available Resources	What is the time-line for completing the study?
	What is the in-house available expertise?
	What expertise can be sub-contracted?
	What potential for external funding is there?
	What are the most critical criteria of the study?
23 Determine Relative Importance of Factors	What factors of functions 21 and 22 are must-haves or just good-to-haves?
A3 Determine Differentiation Approach	How is differentiation going to be achieved?
31 Crosslink Differentiation and Approach Criteria	How do the differentiation requirements relate to available approaches?
32 Identify Approach to Adopt	Which approach satisfies the most differentiation criteria?
22 Malidate Oleaine of America al	Does the selected approach satisfy the study requirements?
33 validate Choice of Approach	Are there any differentiation requirements that have not been achieved?

Figure 5: Summary questions used in Model

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Table 1: The differentiation characteristics of the four main approaches outlined in literature.

Source of Contamination	Nitrate Isotopes	Genetic Markers	Micro- biological	Chemical Markers
Manure (organism 1)		1		
Manure (organism 2)		2		1
Manure (organism x)	1	3	1	
Raw Sewage		4		2
Treated Sewage		4		3
Nitrate in precipitation	2			
Nitrate in fertiliser	3			
Soil nitrogen	4	NA	NA	NA
Desert nitrate deposits	5			
Ammonium in fertiliser	6			

In addition to the differentiation potential of the various approaches, a number of other considerations are of importance in determining the most suitable approach for a particular scenario. These are largely operational parameters. The most pertinent are outlined in Table 2, and the corresponding characteristics of the four main approaches are given. Of note is that certain factors, such as cost and technique availability, may be subjective depending upon the entity carrying out the study. This difference is mainly related to in-house expertise as compared to sub-contracted analyses. Similarly, the level of expertise required might not be considered as important in a particular scenario, as an `expert' in a particular area requiring a high level of expertise may be employed within the entity itself. Furthermore, where sample volumes are given, these are based on the most commonly applied technique to date.

Table 2: Characteristics of the four main approaches. An increased number of '+' symbols indicates an increase in cost, time, level of expertise, state of approach, sample volumes and technique availability.

Table 1). Thus, it is likely that the available resources and approach characteristics are the determining factors in identifying the most suitable approach to be adopted. In this case, it is most likely that microbiological analysis, involving the determination of fecal indicator bacteria (e.g. fecal coliforms) is used. This is because this method is relatively low cost, requires a low level of expertise for its application, is a well-defined approach and is a widely available (routine) technique. However, it has significant time constraints, in that these methods are culture-based. Therefore, sufficient time for

	Nitrate	Genetic	Micro-	Chemical
	Isotopes	Markers	biological	Markers
Instrumentation	IRMS	Various	Incubator	Various
Multi-Source determination	No [*]	Yes	No	Yes
Time requirement	Days	Hours	Days	Hours
Sample Volume	Millilitres	Millilitres	Centilitres	Litres
Typical Cost	++	+++	+	++
Level of Expertise	++	+++	+	++
State of Approach	+++	+	+++	++
Technique Availability	7+	++	+++	++

* Main source or average of the various sources determined.

This supporting material would, therefore, be used in conjunction with the IDEF0 model developed to facilitate the selection of the most suitable approach to achieve nitrate source differentiation. Taking the example of a scenario where the presence of fecal contamination is to be identified, all four approaches would be suitable (

culture growth is required before results can be obtained e.g. 24 hours for fecal coliforms, with limited opportunity for sample storage. On the other hand, if time is deemed a more critical differentiation criterion than e.g. cost, one of the other methods might be more suitable.

Model EvaluationModel verification was the first step in the model evaluation process. Verification ensures that no gaps are present in the model and that consistency is ensured in the ICOM arrow depictions. This factor is particularly critical for those ICOM arrows linking to a parent box and, therefore, needing to be depicted on the corresponding child diagram. Model verification was achieved through the construction of four matrices for the inputs, outputs, controls and mechanism arrows (Tables S.1 – S.4). Each input, control, output and mechanism arrow was represented within its relevant matrix, and it is followed through the hierarchical model. Therefore, if the input arrow I1 is shown on the parent-diagram A0 entering the A1 function box, the presence of the I1 input arrow in the A1 child-diagram is ensured. Within this model, since there is only 1 parent diagram (A0), only one set of matrices was required in order to ensure consistency in the ICOM arrow depictions throughout the model.

Model validation was then carried out. A limited validation of the model is presented here, rather than a comprehensive case study validation, where a particular organization follows the entire decision-making process. Model validation was, therefore, achieved through a series of stakeholder interviews to explore the potential and limitations of the developed decision tool. This included a discussion of the stakeholder's currently adopted approach in scenarios requiring nitrate source determination; the potential for using the decision tool in their organization; the perceived benefits of the proposed decision tool and the perceived limitations of the proposed decision tool. Five individuals from three stakeholder categories within the Irish water and environmental management field were interviewed:regulators, operators and environmental laboratories. The stakeholders interviewed included a river basin district (RBD) coordinator; two county council officials (a scientist and an engineer) within the environmental department; the head of environmental enforcement at a major water and sewerage provider, and; the managing director of an environmental laboratory.

The survey strategy adopted was that of face-to-face semistructured interviews. These are widely used in exploratory and explanatory research, such as that carried out here, since they allow for probing answers and clarifications during the survey process.⁸ An interview pack consisting of the IDEF0 model, the supplementary material, the model's flow chart summary, a reporting tool based on the model's question-based summary and a consent form was used during interviews. These materials, with the exception of the consent form, represent those that will be used for decision tool dissemination. Thus, stakeholder attitudes to the decision tool, as it will be disseminated, could be obtained.

A mixture of one-to-one and group interviews was undertaken, depending upon the interviewees' availability and setting. All interviews were audio recorded following an initial short explanation of the purpose of the interview and the provision of ethical consent. Audio recording allowed for a full record of the conversation to be maintained whilst allowing for increased engagement with the discussion, as compared to extensive note-taking.⁸

From the interviews carried out, it was identified that very little effort has been made in the field of nitrate source determination to date in Ireland. Where it has been carried out, this has largely been in a superficial manner, for example, the identification of risks for nitrate inputs or the use of simple inorganic markers. This scenario is evidence of a significant mismatch between technical advances in the area and what is being used in the field. In fact, it was mentioned that the availability of such a tool is of benefit to the stakeholders, as it allows for the current state of knowledge in this area to be distilled and effectively communicated to the individuals who need to use it, which has been a limitation to date. This outcome indicates that there needs to be increased communication of the potential approaches that may be adopted for nitrate source determination and the advantages and

limitations of the same. The use of this decision tool in the identification of diffuse sources of nitrate contamination seems to be particularly pertinent for the various organizations. Indeed, diffuse nitrate source determination was recognized by most interviewees as a major factor contributing to the tool's potential, as it seems to have been largely ignored to date.

The availability of a decision tool for nitrate source determination was perceived to provide a number of additional benefits to all the stakeholders interviewed, particularly as it allows for a streamlined and more objective thought process leading to the identification of the most suitable approach for differentiating sources of nitrate contamination. Furthermore, it allows for standardized data and, thus, comparisons between studies to be made. In fact, the lack of such a decision tool was identified to have hindered the selection of suitable action plans for environmental remediation and policy development. The format of the decision tool was also mentioned to be userfriendly.

Yet, a number of limitations were also identified through the stakeholder interviews. Some were immediately fed back into the development of the modified decision tool presented here. However, others could not be directly tackled. These include the requirement of specific legislation requiring environmental forensics studies and the development of decision tools for alternative parameters, which may be of greater interest to their specific organization. At the same time, the latter issue shows the interviewee's recognition of the importance and relevance of this tooln the area of nitrate source determination.

Conclusions

In conclusion, technical advances in the field of nitrate source determination have occurred steadily in recent years, particularly in relation to the use of isotopic, genetic and chemical markers. Yet, these techniques have largely failed to transition from academic studies into their application within the field. A reason for this lack of transition is believed to stem from the highly fragmented nature of knowledge in the area, which is approach dependent.

Therefore, this study was undertaken to develop a decisionsupport tool for nitrate source determination and evaluate its applicability through interviews with key stakeholders. The IDEF0 modeling system was used for the decision tool's development in order to ensure the tool's robustness. This IDEF0 model was then translated into a simplified flow-chart to facilitate the model's application since most stakeholders would not be familiar with IDEF0 techniques. In addition to this, supporting material and a reporting tool were developed in order to further facilitate the model's application.

Through interviews held with key stakeholders, it was identified that there is, indeed, currently a need for such a decision tool to support environmental forensics studies for nitrate contamination.. The tool's flexibility allows it to be utilized for a range of purposes, e.g. it can be used in determining a single source of nitrate contamination, or even multiple sources, depending upon the user's requirements. The use of the tool to identify the most suitable approach for diffuse nitrate source determination and fecal contamination were widely recognized as some of the major application of the decision tool. The potential for standardization and objectivity in determining the most suitable approach in nitrate source determination was an additional benefit that was mentioned. This increasing potential is particularly in view of the ever increasing number of numerical models being developed where data from different sources is plugged in, which is currently resulting in incompatible results.

These findings suggest a number of important implications for practice. They identify that there is a definite need for the development of such decision tools in the area of environmental forensics in order to act as a bridge between the current state of technical knowledge and practice. In fact, a number of stakeholders outlined their need for additional tools, depending upon their current requirements. One issue that was not addressed within this study was where would the responsibility for updating the supporting material forming part of the decision tool lie. Whilst the general framework is not expected to require significant updating, the supporting material needs to be reviewed on a regular basis following technical advances in the various fields.

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