NATURAL ENVIRONMENT RESEARCH COUNCIL

Science Programmes — Interdisciplinary Science — Environmental Mathematics & Statistics

EPSRC

WORKSHOP REPORT

Inter-disciplinary workshop on Environmental Remediation

St. Catherine's College, Oxford

24-25 September 2003

Hosted by the University of Oxford in association with the Smith Institute and FIRSTFARADAY

Funded by NERC and EPSRC

Organiser: Dr Andrew Fowler, Oxford Centre for Industrial and Applied Mathematics

FIRSTFARADAY	University of Oxford	Smith institute for industrial mathematics and system engineering

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1. Introduction

A two-day interdisciplinary workshop was held at St. Catherine's College, Oxford on 24-25 September 2003 to bring together mathematicians, statisticians and environmental scientists with the aim of addressing key challenges in environmental remediation. The workshop forms part of an Environmental Mathematics and Statistics thematic programme to fulfill the NERC aim of attracting mathematicians and statisticians to play a more active role in environmental research and to support the EPSRC strategic interdisciplinary priority of environmental mathematics and statistics. In particular, 'the programme is intended to develop rigorous mathematical and statistical reasoning and to bring them to bear on challenges in the environmental sciences.'

The workshop sought to support inter-disciplinary activity between the scientific domains of two Faraday Partnerships and to draw on their experience of collaborative research. The FIRSTFARADAY Partnership[1] aims to bring new science and technology to bear in remediation of contaminated land and water. It has identified a growing future requirement for soundly based environmental risk assessment and for detailed modelling of the processes of contamination and remediation. The Smith Institute Faraday Partnership has a long-term strategy for applied mathematics research that is centred on six themes[2]. The development of greater understanding through the mathematical modelling of processes and the need for the combination of statistical and deterministic techniques are issues which are, respectively, at the heart of the themes of simulation and uncertainty and risk.

The workshop benefitted from the natural synergy in long-term research aims of the FIRSTFARADAY and Smith Institute Industrial Mathematics Faraday Partnerships, brought together researchers to initiate and pursue inter-disciplinary activity in mathematics, statistics and environmental science.

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[1] http://www.firstfaraday.com/
[2] www.smithinst.ac.uk/news/RoadmapLaunch

2. <u>Workshop objectives</u>

The aims and objectives of the workshop were to:

- Stimulate the application of mathematics and statistics to challenges in environment science
- Increase the proportion of each community collaborating in the long term
- Identify opportunities for research proposals in adjunct disciplines
- Catalyse the formulation of new interdisciplinary project teams

3. <u>Workshop structure and session titles</u>

The workshop was structured according to a Study Group format established and used by the Industrial Mathematics community in the UK for over 30 years. Three topic areas were presented to the workshop attendees as one-hour talks with question and answer sessions for clarification.

To discuss the topic areas in more detail, the attendees split into three breakout sessions in different rooms each with a moderator and a facilitator. Each session topic was debated in more detail, with the facilitators taking notes and the moderators providing a loose steer. Although the structures of the breakout sessions were left open, they broadly followed an initial investigation by the mathematicians and statisticians who questioned the environmental scientists to ensure that they understood the issues. This was followed by further discussion on the area of interest and the key questions / problems. Finally, the potential opportunities for mathematics and statistics to contribute to the area of environmental remediation were formulated and the basis of future projects and collaborations was established.

To focus on specific areas of need, highlighted by the FIRSTFARADAY team, the issues raised by three key challenges in environmental remediation were discussed :

- Propagation of uncertainty for decision making in environmental remediation
- Sampling strategies and data fusion and data gathering in environmental risk assessment
- Modelling and simulation for process design and assessment: a permeable reactive barrier for pathway treatment

4. Workshop session 1. Propagation of uncertainty for decision making in environmental remediation

Presented by: Professor David Lerner, University of Sheffield
Moderators: Dr Peter Craig, University of Durham and Dr Lenny Smith, London School of Economics
Facilitators: Dr Tim Boxer, Smith Institute Faraday Partnership, Perry Guess, FIRSTFARADAY partnership

Background: The key to decision making in environmental remediation of a site is quantifying the uncertainty in the risk assessment and establishing the confidence requirements of each stage in the process. At present the risk is assessed using a process with broadly three stages: (i) use of knowledge of the site history (ii) further data gathering and uncertainty estimation in the light of the new data (iii) conceptual modelling of processes of pollutant evolution and remediation. The models in stage (iii) range in complexity according to need, including simple algebraic models, 1d transport models and bespoke CFD. If the uncertainty is small enough at the end of any stage then a decision can be made about the risk posed and the analysis is taken no further.

Challenge: To examine and propose improved mathematical and statistical methods to quantify required confidence levels and propagate uncertainty at each stage in the assessment process up to the point of decision making. The overall process of specifying confidence levels and marshalling uncertainties in the assessment of risk will be examined. For example, in the first stage the formulation of prior probability density models may be examined, drawing on experiences in the oil industry. For the second stage the confidence levels required of sampling strategies will be examined. At the third stage some statistical methods are already in use but there is a need to understand the requirements for the combination and improvement of deterministic and stochastic elements in the model.

Workshop report:
To maximise the chance of identifying technology transfer opportunities from the oil industry to the environmental remediation industry the discussion mainly focussed on those contaminated land sites for which the data available is comparable with that available for oil fields. More geophysical data can be afforded for risk assessment of sites with significant size and importance that would be costly to remediate. Groundwater remediation by pump and treat in fractured bedrock on significant sites provides the closest analogy to the oil industry and was the example used to motivate discussion of the suitability of various modelling approaches.

- **Support of decision making**

- *Which decisions*? Risk assessment / sampling decisions / cost-benefit analysis (including costs and benefits of additional calculations).
- *Who need to be satisfied with model*? Regulators, insurance companies, land owners.
- *What are the design considerations*? Flow, biodegradation, dispersion, adsorption, heterogeneity, cost, etc…
- *Is it sensible to expect the model to predict the breach of a threshold*? Maybe an order of magnitude prediction would be more appropriate (logarithmic scale).

The scope of the model should be defined according to the information required from the model output. This requires a dialogue between the regulators, environmental assessors, environmental scientists, mathematicians and statisticians. Given the current limits of technology and understanding the level of model accuracy desired may not yet be feasible. A challenge lies in assessing the marginal value of additional modelling and analysis before incurring the associated costs.

➢ **Increased accuracy in predictive modelling for risk assessment**

- *Do we wish to continue with current models that overestimate the risk*? Current models are considered to be conservative, but this statement can only be supported by first quantifying the uncertainty.
- *Would we rather have a predictive model that aims to provide an accurate assessment of the risk*? In which case it is more important to understand the uncertainty in the model predictions; a less conservative approach raises the probability of predictions that underestimate the risk.
- *Is it acceptable to have models that sometimes underestimate the risk*? The costs of poor decisions need to be included to do the full cost-benefit analysis.

Attempts to improve model accuracy must be supported by quantification of the uncertainty in predictions. For these predictions to be accepted they must support the total cost-benefit analysis which includes the costs of both overestimation and underestimation of the risk. There are opportunities for technology transfer from the oil industry in this area.

➢ **Hierarchical modelling**

- *Can a quantitative model be built up from the conceptual model*? Currently the conceptual model is in the form of a diagram built up from site-specific historical data and expert knowledge.
- *What are the important features of the real situation that need to be added to enhance the model and make it more accurate*? Heterogeneity, biodegredation, dispersal, adsorption, advection, cost, etc…
- *What degree of uncertainty is added to the model predictions when these features are added*? Expert knowledge can be used to form prior probability distributions on uncertain initial or boundary conditions and uncertain coefficients.

The aim of a hierarchical approach would be to converge on a more accurate prediction as model sophistication is increased, but also to quantify uncertainty at each stage in a systematic way. Expert knowledge needs to be captured in prior probability distributions to begin to quantify the uncertainty. The equations should be experimentally validated in situations where the input data are known in detail and estimates of the probability of events predicted by the model should be implied by estimates of the input parameters and the equations.

➢ Data uncertainty

- *What are the main things contributing to data uncertainty*? Source size, location and composition; calibration of geophysical data, sample handling etc…
- *Can laboratory measurement be scaled-up with confidence into field data*? Many experiments have shown large differences between in vitro and in vivo.
- *What is the best use of limited data*? Use data to most effectively reduce uncertainty (repeats) or improve resolution (grid points).
- *Can data be used from other similar sites*? This requires care and the use of expert knowledge to assess its value.

Data is available in many forms from expert knowledge, geological observations, on site physical measurements, laboratory measurements, etc… However all information and measurements should be treated as uncertain to some degree. Uncertainty can be reduced through propagation of best practice to reduce error in sample and data handling and through research into new sensors and the relationship between laboratory and field observations. Attempts to apply geophysical technology from the oil industry have highlighted several important barriers to transfer including the different measurement scales and sensitivities involved both spatially and temporally and the lack of financial resources in remediation geophysics.

➢ Quantifying and reducing model uncertainty

- *How can model uncertainty be reduced*? More detailed process modelling and use of more powerful computing and better algorithms to perform the analysis.
- *How can model uncertainty be measured*? Existing methods, applied in weather forecasting and the oil industry, include ensemble forecasting through Monte Carlo simulations of a reduced model (emulator, homogenisation or multi-scale approach) with the same qualitative behaviour as the full model.
- *Should the emphasis of research be on reducing or measuring uncertainty*? A framework for uncertainty measurement needs to be developed for existing models and then applied to improved models as they are developed.

More detailed process modelling is required to describe the phenomena more accurately and greater insight needs to be gained into the qualitative behaviour of existing and future models to help build approximations and emulators. The difference between the natural world and both model inputs and outputs needs further modelling. A better framework needs to be developed for assessing uncertainty in current and future models. Research into new techniques in these areas would be needed to address the specific challenges faced in environmental remediation.

Proposed research agenda

1. Identification of technology transfer opportunities to and from the oil exploration and environmental remediation research communities;

2. Translation of expert knowledge by environmental scientists into statistics to define prior probability distributions on model inputs;
3. Development of efficient methodologies to calculate risk sufficiently accurately from the posterior probability distributions that derives from the prior distributions and data to be assimilated.
4. Increase the speed of data assimilation through the use of emulator models, multi-scale methods or homogenisation techniques.
5. Convergent hierarchical modelling: building up from the conceptual model to more detailed process models that can be trusted by decision makers;

Actions

1. Michael Goldstein and Peter Craig, Durham, and Bernd Kulessa, Belfast, have begun discussing the possibility of using statistical methods to integrate the results from different site investigation techniques (incl. geophysics in particular) into one common variable that reflects the (changing) properties of contaminants in the ground. They are aiming to put an EPSRC grant proposal together on this in the near future.

2. Bernd Kulessa and Chris Farmer are discussing the transfer of technologies from the oil geophysics to the contaminated land area.

3. A follow-up study group (1.5 days) is to be held in Oxford in January to focus on three specific site problems involving reaction schemes which have been encountered by David Lerner and colleagues in Sheffield. The aim will be to look at the complex chemistry and to reduce, simplify or reformulate the problem to one that is computationally more feasible.

5. Workshop Session 2.

Sampling strategies and data fusion for data gathering in environmental risk assessment

Presented by: Dr Paul Nathanail, University of Nottingham
Moderator: Professor Michael Goldstein, University of Durham
Facilitator: Melvin Brown, Smith Institute Faraday Partnership

Background: For improved risk assessment and the verification of environmental remediation, more quantitative and holistic approaches are needed in the design and collection of data to ensure the achievement of pre-defined levels of confidence in the data obtained. Improvements in the use of statistical planning techniques will reduce the sampling effort required and the use of models of physical processes to inform the sampling strategy will address the challenges posed by heterogeneity of source positions in particular.

Challenge: (a) To review and propose improved systematic methods of data fusion to enable the combination of various quantitative measurements made on site, results of analyses made in the laboratory, the effects of environmental conditions, observations from non-quantitative sources such as field records and photographs, and inferences from models of physical and biological processes (b) To examine and propose new sampling strategies using statistical planning techniques and data fused from many sources to optimize the sampling effort and secure the confidence levels required.

Workshop report:

Introductory discussion

- Focus on processes for addressing and answering the question: To remediate or not to remediate?
- How is the evidence assembled and marshalled to the point of decision and, given the evidence, what are the factors (and their significance) affecting the decision?
- Evidence comes from many sources: experts, maps, historical documents, measurements (past), measurements (to be taken?), various levels of site survey, detailed models, less detailed models. Is there a common framework into which such data may be fused?
- How to decide what information to collect and how much? 'Where to draw the line?'
- What is the marginal value of the information in the decision making process? This is important in making decisions about courses of actions and their 'effectiveness' not in themselves but in the context of the decisions that have to be made.
- How to recognise and treat rogue data?
- How can the information (prior and additional) and decision making process be assembled into a logical structure? A mechanism is required to evaluate the likelihoods of possible states and to combine them with utility

of those states to all the players – Environment Agency (EA), insurance companies, developers, landowners, etc

- How do we include the costs of possible courses of action during the assessment process?
- Projecting into the decision space: what are the dimensions of that space**?**
- **Suppose we use Bayesian methods and networks, hereafter the Bayesian Framework (BF).**

Examples

- **Gas works:** Similarity to other site of same kind? Value prior information - how many new samples would you trade for the prior? How to elicit information from experts and convert it into priors in the BF? Ask different experts? What is the return (units?) on the cost of more experts, code analyses, measurements?
- **Garden:** How can the BF handle spatial data? Independence of sources of information: e.g. what is the covariance between samples taken at different locations – use related parameters eg pH. How to choose a sampling strategy? Use (somehow consistently) existing data (from EA, codes, etc) on gardens to inform strategy. Need to have consistent way of including information from earlier 'tiers' even if it was insufficient to make decision at those earlier stages. How do we know that the contractors faithfully carried out the sampling task? … Ask for repeated data and report … but what is it worth? What about the concerns of the neighbours – why not dig up their gardens – the whole street!
- **CHP:** Stages: 1) Outline application – what do we need to protect 2) Conceptual model: sources, pathways, receptors 3) Common features from other sites 4) Site survey – walk over – shallow trenches for top soil sample…

Applying a Bayesian Framework

Prior probability for this type of site	**Actual state**	**~Test/survey suggests OK**	**~Test/survey suggests not OK**
30%	**Site OK**	**90%**	**10%**
70%	**Site BAD**	**30%**	**70%**

- Observing the results of the test/survey allows evaluation of **P(Site OK | result of test)** and **P(Site BAD | result of test)** by use of Bayes theorem, given the respective prior probabilities.
- Use utility/reward functions (U) for the state of the site and the courses of action:

Action	**Actual state OK**	**Actual state BAD**
Do nothing	**U1**	**U2**
Remediate site	**U3**	**U4**

- The expected utilities are then

  U_N (Do nothing) = U1*P(site OK|result of test) + U2*P(site BAD|result of test)
  U_R (Remediate) = U3*P(site OK|result of test) + U4*P(site BAD|result of test) .

  The decision goes to: **max (U_N , U_R) ,** ie this is 'where the line is drawn'.
- The challenges of the Bayesian approach are therefore: (i) to get realistic prior probabilities for the different states (ii) to get make accurate assessments of the probabilities of the data given the different possible states of the site (respecting the temporal and spatial aspects of the problem) (iii) to form a meaningful utility table respecting the values of each consequence to all of the protagonists. Having constructed these ingredients, then all other aspects of the problem, such as how much information does any given sampling scheme provide, how can we achieve maximal information for minimal cost, how can we weigh sampling costs against costs of bad decisions, etc. follow by straightforward calculation.
- Input of science affects the probabilities and utility function theory allows the combination of different attributes to form overall utilities in the final decision space. Bayesian networks allow identification and collation of independent and dependent sources of information. The framework might allow determination of decision sensitivities to changes in the Ps and Us, both as the decisions on courses of action during the site assessment process are being made and also provide an audit trail for the final decision. The framework also tempers the influence of ad hoc decisions - they are margin pulls.
- Issues of knowledge elicitation from different sources and their fusion need to be addressed.
- Further discussion of how to handle spatial correlations between sample points: point has mean and variance and off diagonal of VCV matrix can use $\exp(-(R_{ij}/a)^2)$, R_{ij} separation of sample points i and j and 'a' a correlation distance determined by modelling.
- Can the existing regulatory framework accommodate the use of a Bayesian Framework in the context of the session challenges[3]?

[3] Post-meeting note by Bob Barnes of Environment Agency: A bayesian framework would be a statistical tool to aid in decision making and would (hopefully) provide greater confidence that the correct decision was being made based upon an adequate characterisation of a piece of land. The issue of whether to remediate or not would depend upon the remedial goals which in turn are based upon the regulatory driver relevant to the site. The Contaminated Land Regulations relate remedial objectives to the current use of the land and the need to remediate to prevent significant harm or the significant possibility of significant harm or pollution of controlled waters. The Planning Regime (explained in Planning Policy Guidance Note 23) requires land to be "suitable for use" - risks should be assessed and remediation requirements set on the basis of both the current use and circumstances of the land and its proposed new use. In both instances the risk management framework is contained in the joint DEFRA, IEH and Environment Agency publication "Guidelines for Environmental Risk Assessment and Management" (2000) known as Greenleaves 2; and specifically for land contamination within the draft Agency publication "Model Procedures for the Management of Land Contamination (CLR11). This implies a tiered, site specific risk assessment and the use of a Bayesian Framework would fit with the requirements for site characterisation within the assessment.

Notional research agenda and collaboration

- Review of 'state of art' for application of BF to environmental remediation is required to establish the 'ground' of a valid research agenda.
- Develop methodology around real cases, 1) first at a crude level to draw out all issues and then in more detail to test practicality of approach. 2) Identify and follow-up key research issues (eg elicitation from experts and codes, maps etc and integration into BF) 3) Develop prototype software to implement methods and apply to the case data (EA data acts as 'blind test') 4) beta test the method/software on real study carried out by EA consultants 5) Must use diverse case studies.
- Potential collaborators: **Environment Agency of England and Wales** – supply of historical case study and provide opportunity to beta-test methods/software on real cases. **Shell** - provide site data (maps, standpipes, boreholes, geology/soil etc) from 2-3 storage tank farms as examples of 'localised' sources. **IGER** (**CI**)– provide data/case studies for 'nonlocal' sources eg nitrogen/agricultural sources. **Durham (Statistics) (PI)** host 3yr post-doc in statistics: 1) Learn characteristics of domain data and issues, 2) adopt/develop statistical methods for sampling, elicitation, fusion and decision making framework, 3) implement methods in software and test against case studies (historical and live). **Durham (Geology) (CI)** host 3yr CASE PhD (with geological science background) with **Shell** . CASE student to work at the modelling level to support the methodological emphasis of the post-doc. Focusing perhaps upon one set of case data. (PhD title: Modelling contaminated land assessment using Bayesian methods).
- Funding: Need to identify funding sources NERC/EPSRC. Smith Institute could participate if separately funded to provide project management/technology translation.

Actions:

1. Clive Anderson has approached Chris Farmer (Schlumberger) regarding potential collaboration.
2. Michael Goldstein to draft outline statistics post-doctoral proposal to research and develop a Bayesian framework for environmental remediation, involving Kit Macleod (IGER) and Fred Worral (Geology) at Durham and making use of data provided by Shell and Environment Agency (Bob Barnes).
3. Maggie Wenham (Shell) to explore possibility of CASE student with Durham (geology) to run alongside 2 above.
4. Smith Institute and FIRSTFARADAY to seek mechanisms for funding their support to collaborations and future activity

6. **Workshop session 3.**

<u>Modelling and simulation for process design and assessment: a permeable reactive barrier for pathway treatment</u>

Presented by: Dr Norman Kirkby, University of Surrey
Moderator: Dr Andrew Fowler, University of Oxford
Facilitator: Dr Simon Jackman, FIRSTFARADAY partnerships

Background: The use of a Permeable Reactive Barrier (PRB) may be required to intercept a groundwater pollutant plume if monitored natural attenuation (MNA) is an inadequate remediation process. When plumes contain a complex mixture of contaminants, these may require several separate treatments (chemical and microbiological) within the same PRB to treat all of the contaminants. The design of these barriers becomes complex in comparison to traditional chemical catalytic or sorptive PRBs and there is therefore a requirement here for the use of detailed modelling to inform the design of remediation processes and strategy.

Challenge: To demonstrate how simulation through mathematical modelling and analysis can be used to develop understanding of the processes involved. A particular next generation robust PRB will be analysed. The modelling required is of microbiological process, hydrogeological process, groundwater flow and reactions. The study will show how the analysis of sensitivities to perturbations can aid the design of robust PRBs. The integration of measurements of the MNA of the site with deterministic aspects of the modelling in order to predict the attenuation of pollution will be examined. An important aspect will be evaluation of the statistical significance of the contribution of the barrier to the site remediation.

Workshop report: Discussion within the workshop focussed on the complexity of biological systems and the necessity for simple modelling approaches in order to understand the connection between changes in biological parameters and effects on the biodegradation of contaminants.

The discussion followed Norman Kirkby's presentation of microbial systems and the complexities of understanding growth and metabolism in the context of different bioreactor systems in which conditions such as dilution rate, substrate concentration or other parameters such as pH are maintained at a constant level. The genetic switches that direct cell growth, stasis and apoptosis are not yet fully understood and yet these are vital controls to the formation of appropriate in situ bioreactors for the treatment of contaminated groundwater. There is therefore a requirement to understand these processes and their controls before predictive modelling can be performed.

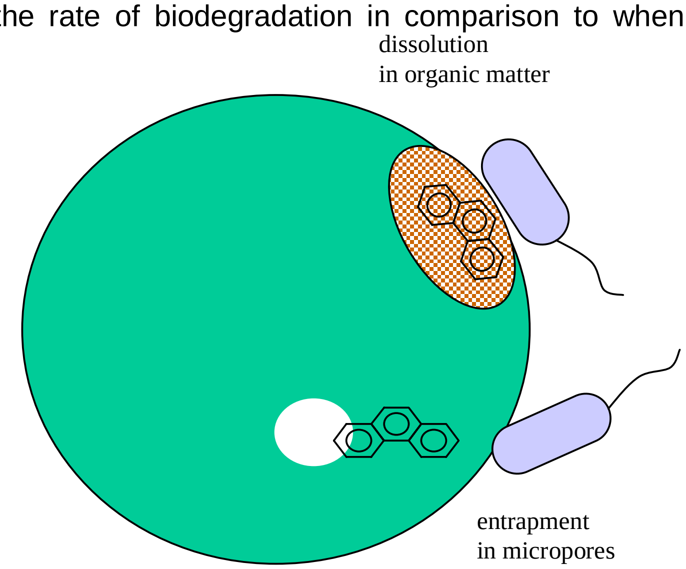
In order to commence the engagement between the two communities of environmental scientists and mathematicians / statisticians, two simple example systems were presented. These reflected the two situations presented by Paul Nathanail and David Lerner, in dealing, respectively, with contamination in the unsaturated zone, the degradation of which is affected by bioavailability, and that in a plume within the saturated zone, where degradation is affected by transport, sorption and biodegradation processes.

The Unsaturated Zone – Bioavailability

The bioavailability of contaminants to microbes can be described as the amount or proportion of the contaminant that is accessible to the organisms for metabolism. When a soil is contaminated, there is frequently an initial degradation of the contamination by indigenous microorganisms. Over time, however, the contaminant becomes aged within the soil and is no longer available for microbial transformation. The ageing process can be summarised in a number of sub-processes including dissolution in soil organic matter, ionic or hydrophobic binding to soil components or encryption within soil micropores. A combination of these processes, and others, frequently lead to contamination remaining in the soil with the potential of residual risk and potential impact upon human health and the environment.

In order to tease apart the individual processes contributing to bioavailability, microbiologists are developing model systems in which many of the parameters are kept constant, allowing individual parameters to be varied and their overall contribution to the effect to be elucidated. One such model system uses polymeric beads to represent different compartments (e.g. hydrophobic, ionic and micropores). By using a single species of bacterium and a contaminant which it is able to degrade, it may be possible to establish the mass transfer limitations to biodegradation and how these are affected by environmental conditions (e.g. pH, ionic strength, surfactants etc.).

The Oxford team (Simon Jackman and Chris Knowles) have been working on polymeric beads with the contaminant 3-chlorobiphenyl, a polychlorinated biphenyl. This has been sorbed to 3 different polymeric bead surfaces and *Burkholderia* sp. LB400 was added to the beads. With the hydrophobic bead surface, biodegradation of 3-CB to 3-chlorobenzoate was mass transfer limited. In contrast, sorption to an ionic (anion exchange resin) bead did not reduce the rate of biodegradation in comparison to when the 3-CB was in solution.



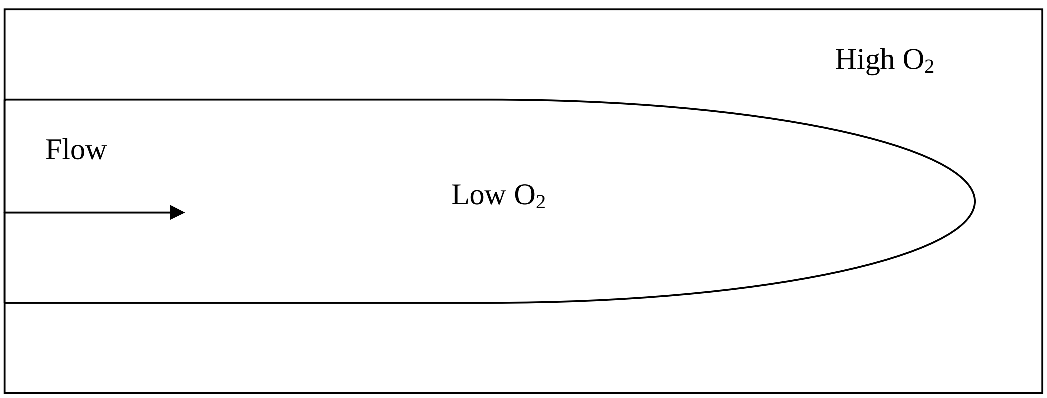
In the figure, bioavailability can be controlled by dissolution of the contaminant in organic matter, leading it becoming unavailable to bacteria, or entrapment within micropores, also leading to a lack of bioavailability.

With this system, there is a requirement to vary the intrinsic parameters, including using particles of different pore sizes and surface properties. Microbial adhesion processes may also be contributing to their ability to degrade the contaminants.

Can the complete system be modelled using a 1-dimensional diffusion model that assumes that diffusion in the bacterial membrane is the primary mechanism for uptake of the contaminant for biodegradation ?

The saturated zone – porous flow and biodegradation

David Lerner has developed a model aquifer system incorporating a monolayer of glass beads between two glass plates. This is perfused with buffer and inoculated with bacteria capable of degrading acetate. The buffer incorporates an indicator fluorescent dye indicator for oxygen. In the absence of oxygen, the dye changes colour, indicating the utilisation of acetate. The system has been analysed by CCD photography and a mathematical model has been applied to the system to incorporate flow dispersion and advection and biodegradation using Monod kinetics derived from batch culture experiments.



The challenges of this system are to increase complexity to microbial consortia, multiple contaminants with different flow properties and to use different indicators to link more directly to microbial metabolism of contaminants.

Issues of bacterial growth and clogging of pores have yet to be assessed within aquifer flow systems, therefore this may be of interest to be investigated within a model aquifer. The balance between growth and mineralisation could be investigated.

Other ideas included the investigation of alternative electron acceptors, the use of pulsed flow to visualise oxygen replenishment of deprived areas as a method to assess the rate of oxygen diffusion and laser bleaching to achieve much the same effect. A plug flow system would also enable the detection of exit concentrations of acetate and oxygen, leading to an estimate of the mean rate of consumption of acetate. It would also be of interest to investigate a non-degraded substrate and its effects upon bacterial metabolism.

Actions

1. Andrew Fowler, Simon Jackman and Andrew Singer are generating a proposal for an EMS studentship to focus on modelling of bioremediation and bioavailability.

2. Andrew Fowler and Simon Jackman are to organise a group discussion with Andrew Singer, Peter Howell, Norman Kirkby and Chris Knowles to address the modelling of complex cellular and environmental processes, together with Tiina Roose and Arun Mudiganti.

3. David Lerner and Andrew Fowler are discussing a potential studentship on modelling of plume dynamics in a model system.

4. Norman Kirkby is to meet Marcus Tindall from the Centre for Mathematical Biology in Oxford to discuss cell cycle modelling and potential ways forward, bringing together a biochemical engineer and a mathematical biologist.

6. Outcomes and future directions.

The workshop was very well received within both the Mathematics and Statistics communities and in the Environmental Sciences community as seen from the list of delegates (see Appendix) all of whom attended.

A number of the delegates had not previously been involved with members of the other community and therefore this was an excellent opportunity to start building together a cohesive approach to tackling complex environmental problems with mathematical and statistical approaches.

Real challenges were presented and approaches were formulated. In particular, from workshop 1, the potential for transfer of techniques from the oil and other industries to provide a framework for the quantification of uncertainty in risk assessment, from workshop 2, the potential application of a Bayesian framework to data analysis/fusion and decision making in environmental remediation, and from workshop 3, the use of simple models for interrogating the interactions at a molecular and cellular level that underpin the bioremediation of contaminated land.

Projects

Opportunities for multidisciplinary multi-stakeholder research proposals were identified in each area. In particular:

- An EPSRC proposal on geophysical techniques
- A potential post-doctoral project and a CASE studentship on a Bayesian framework for environmental decision-making
- A larger project with the regulator, a site owner, statisticians and geologists to develop a Bayesian framework for contaminated land
- An EMS studentship on modelling bioavailability
- An EMS studentship on modelling natural attenuation in a model plume

Each of these potential outputs will involve the formation of new project teams.

Networks

At a strategic level, there is a significant requirement for mathematical and statistical approaches to be applied to the environmental sector. This was identified as the reason behind the workshop. Whilst the workshop has served to take collaborations forward to a new level, there remains a large amount of work to be done in establishing a momentum in the these communities to ensure the benefits of interaction are embedded within the infrastructure. The ongoing development of the communities could best be facilitated by the development of networks, an EPSRC-funded **R&D network** to draw together the academic communities, and a DTI-funded **best practice network** to ensure that the developments in the research community are linked to implementation by the industrial community that puts environmental tools into practice. FIRSTFARADAY and the Smith Institute together could play an important role in leading a future programme of activities to build on the outcomes from the workshop, given mechanisms to support their ongoing participation.

Training
Opportunities exist for the training of both communities, through studentships and discipline-hopping awards, but also through training courses that may be developed to ensure that the environmental science community is able to use the mathematical and statistical tools that are available and that they understand how to access higher level input when required.

7. Funding Opportunities

Details of funding opportunities were presented to the workshop participants by Allison McCaig of the Mathematics programme within EPSRC.

The Environmental Mathematics and Statistics (EMS) programme is a capacity building initiative with a budget of £ 3.5M. It is designed to enhance the quality and quantity of collaborations between the mathematical/statistical and life science/environmental communities and to support and develop a community with the skills needed to use novel mathematical/statistical techniques to address problems in environmental science. Its final aim is to stimulate research and submission of proposals at the environmental/mathematical science interface.

With this in mind, the **EMS programme** has the following funding opportunities:

1. Studentship (25) with a £4K stipend enhancement (deadline 15 November 2003)
2. Discipline-bridging awards (6)
3. Postdoctoral fellowships (1; deadline 21 November 2003)
4. Workshops/courses (8; deadline 5 December 2003)

In addition, **EPSRC** has the following funding mechanisms that are not directly focussed on the EMS programme:

1. Responsive mode grants
2. First grants for new academics
3. Mathematics small grant scheme (< £10K)
4. Workshops/symposia
5. Fellowships

    A. Postdoctoral (mathematics) – 3 years (deadline 13 October 2003)

B. Advanced/senior (cross-EPSRC; deadline 14 November 2003)

C. European young Investigator (EURYI; deadline 15 December 2003)

6. Mathematics CASE projects (call in October 2003)

7. The Mathematics Underpinning Life Sciences initiative of the EPSRC funds novel mathematics and statistics that address problems of relevance to the life sciences. There is joint funding between the Mathematics and Life science interface programmes. At least 50 % of the research has to be within the EPSRC remit. Outline proposals are welcome in this area.

8. Research Networks are designed to promote the transfer of knowledge and encourage collaborative activity. They encourage research collaborations between mathematics (including statistics) and other disciplines and non-academic organisations. Funding of up to £ 60K is available over a 3 year period.

The **LINK Bioremediation** programme is funded by DTI, BBSRC, EPSRC, NERC, MRC, ESRC, Environment Agency of England and Wales and the Scottish Executive Environment and Rural Affairs Department (SEERAD) to support the development of technologies that will provide UK industry with the multidisciplinary capability necessary to enable the commercial exploitation of biotechnology for the clean up of contaminated land, air and water. Funding of up to 50 % of eligible costs is available for pre-competitive projects between industry and academia. The closing dates for outline proposals are 13 February, 3 June and 3 October 2004.

Training opportunities

1. Short instructional courses in mathematics and statistics (sponsored by EPSRC) to broaden the mathematical skills of first and second year PhD students are available from the London Mathematical Society (www.lms.ac.uk) and the Royal Statistical Society (www.rss.org.uk).

2. Mathematics for engineers is a joint initiative between the Mathematics and Engineering programmes. Pilot course in mathematics for acoustics and process engineering have been conducted. The aim is to introduce engineers to the range of mathematical techniques. A call for proposals is to be announced in spring 2004.

Public awareness activities

The Public Awareness programme of EPSRC provides Public Communication training funds, partnerships for Public awareness awards, media fellowships and the pupil researcher initiative.

EMS contacts:

NERC: Frances Collingborn (frco@nerc.ac.uk)
Chris Baker (ckb@nerc.ac.uk)

EPSRC: Allison McCaig (Allison.mccaig@epsrc.ac.uk)

Appendix

Participants at Inter-disciplinary Workshop on Environmental Remediation

Participants

Prof Clive Anderson	Department of Probability and Statistics, University of Sheffield	c.w.anderson@shef.ac.uk
Dr Matthew Ashmore	Land Quality Management Scheme, University of Nottingham	Matt.ashmore@nottingham.ac.uk
Bob Barnes	National Groundwater and Contaminated Land Centre, Department of Environment	Bob.Barnes@environment-agency.gov.uk
Dr Ron Bates	Department of Statistics, London School of Economics	r.a.bates@lse.ac.uk
Dr Tim Boxer	Faraday for Industrial Mathematics, Smith Institute	Tim@smithinst.co.uk
Melvin Brown	Faraday for Industrial Mathematics, Smith Institute	Melvin@smithinst.co.uk
Brenda Chisala	University of Sheffield	Eip02bnc@sheffield.ac.uk
John Collins	Department of Geological Sciences, Unversity of Durham	j.p.collins@dur.ac.uk
Dr Peter Craig	Department of Mathematical Sciences, University of Durham	P.S.Craig@durham.ac.uk
Dr Diganta Das	Department of Engineering Science, University of Oxford	Diganta.Das@eng.ox.ac.uk
David Drury	Golder Associates (UK) Ltd	ddrury@golder.com
Dr Andrew Fowler	Mathematical Institute, University of Oxford	Fowler@maths.ox.ac.uk
Prof Michael Goldstein	Department of Mathematical Sciences, Unversity of Durham	Michael.goldstein@durham.ac.uk
Perry Guess	FIRSTFARADAY, Pera	Perry.guess@pera.com
Dr Peter Howell	Mathematical Institute, University of Oxford	Howell@maths.ox.ac.uk
Dr Simon Jackman	FIRSTFARADAY , University of Oxford	Simon.jackman@eng.ox.ac.uk
Prof John King	Theoretical Mechanics Section, University of Nottingham	John.king@nottingham.ac.uk
Dr Norman Kirkby	Chemical and Process Engineering, University of Surrey	n.kirkby@ntlworld.com
Prof Christopher Knowles	FIRSTFARADAY , University of Oxford	Chris.knowles@eng.ox.ac.uk
Dr Bernd Kulessa	School of Civil Engineering, Queen's University Belfast	b.kulessa@qub.ac.uk
Prof David Lerner	Department of Civil and Structural Engineering, University of Sheffield	d.n.lerner@sheffield.ac.uk
Dr Gordon Lethbridge	Shell Global Solutions	gordon.lethbridge@shell.com
Sharron Long	Elsevier/Nottingham University	s.long@elsevier.com
Dr Kit Macleod	IGER	Kit.macleod@bbsrc.ac.uk
Duncan McKnight	Department of Civil and Structural Engineering, University of Sheffield	d.mcknight@sheffield.ac.uk
Arun Mudiganti	BAE Systems	arun.mudiganti@baesystems.com
Dr Paul Nathanail	Land Quality Management, University of Nottingham	Paul.nathanail@nottingham.ac.uk
Dr John Ockendon	Oxford Centre for Industrial and Applied Mathematics, University of Oxford	Ock@maths.ox.ac.uk

Participants (continued)

Dr Martin Paisley	Mathematics and Statistics Division, Staffordshire University	m.f.paisley@staffs.ac.uk
Prof Kevin Parrott	Computing and Mathematical Sciences, University of Greenwich	a.k.parrott@gre.ac.uk
Prof Simon Pollard	Integrated Waste Management Centre, Cranfield University	s.pollard@cranfield.ac.uk
Dr Iead Rezek	University of Oxford	Irezek@robots.ox.ac.uk
Dr Tiina Roose	Oxford Centre for Industrial and Applied Mathematics, University of Oxford	Roose@maths.ox.ac.uk
Dr Graham Sander	Department of Civil and Building Engineering, Loughborough University	G.Sander@lboro.ac.uk
Dr Andrew Singer	CEH Oxford	acsi@ceh.ac.uk
Alan Smalley	University of Sheffield	a.smalley@sheffield.ac.uk
Dr Lenny Smith	London School of Economics	Lenny@maths.ox.ac.uk
Dr Joseph Teer	QDS Environmental Ltd	Joe.Teer@QDSLTD.com
Simon Woodhead	University of Bristol	Simon.woodhead@bris.ac.uk
Dr Maggie Wenham	Shell Global Solutions	Maggie.wenham@shell.com
Dr Fred Worrall	Department of Geological Sciences, University of Durham	Fred.Worrall@dur.ac.uk
Dr Allison McCaig	EPSRC	Allison.McCaig@epsrc.ac.uk
Dr Bruce Malamud	Kings College, London	bruce.malamud@kcl.ac.uk
Dr Chris Farmer	Schlumberger Information Solutions	cfarmer@abingdon.geoquest.slb.com

Participants by discipline

Mathematics

Dr Tiina Roose	University of Oxford	Mathematical biology
Dr Peter Howell	University of Oxford	OCIAM
Prof. John King	University of Nottingham	Theoretical Mechanics
Dr Andrew Fowler	University of Oxford	Environmental Mathematics
Dr Graham Sander	Loughborough University	Civil & Building Engineering
Prof. Kevin Parrott	University of Greenwich	Finite element and volume methods
Dr John Ockendon	University of Oxford	OCIAM

Statistics

Dr Lenny Smith	LSE	Environmental estimation
Dr Peter Craig	University of Durham	adsorption of pollutants on contaminated land
Prof. Michael Goldstein	University of Durham	Bayesian engineering
Dr Ron Bates	LSE	Spatial methods
Prof. Clive Anderson	University of Sheffield	Statistical modelling and inference
Sharron Long	Elsevier / Nottingham	Environmental data quality

Environmental Science

Dr Bernd Kulessa	Queen's Belfast	Geophysical imaging / engineering
Dr Paul Nathanail	University of Nottingham	Environmental risk Assessment
Dr Norman Kirkby	University of Surrey	Modelling biological Systems
Prof. Chris Knowles	University of Oxford	Bioremediation
Prof. David Lerner	University of Sheffield	contaminant Hydrogeology
Prof. Simon Pollard	Cranfield University	Waste technology / risk Management
Dr Andrew Singer	NERC CEH Oxford	Environmental Microbiology
Dr Fred Worrall	University of Durham	Contaminant hydrology
Dr Kit McLeod	IGER	
Dr Matt Ashmore	University of Nottingham	contaminated land management
Dr Iead Rezek	University of Oxford	Modelling with Uncertainty in Biomedical Systems

Dr Diganta Das	University of Oxford	Porous flow modelling
Dr Martin Paisley	Staffordshire University	Environmental data Analysis
Dr Bruce Malamud	Kings College, London	Environmental Monitoring and Modelling

Graduate Students

Simon Woodhead	University of Bristol	NERC/EPSRC student in Statistics/Geography
Brenda Chisala	University of Sheffield	Groundwater modelling
John Collins	University of Durham	Pollutant transport / spatial uncertainty
Duncan McKnight	University of Sheffield	Pollutant transport Modelling
Alan Smalley	University of Sheffield	Pollutant transport Modelling

Industry

Dr Bob Barnes	Environment Agency
Dr Gordon Lethbridge	Shell Global Solutions
Dr Maggie Wenham	Shell Global Solutions
Arun Mudiganti	BAe Systems
David Drury	Golder Associates
Chris Farmer	Schlumberger

Technology Translators

Dr Simon Jackman	FIRSTFARADAY
Perry Guess	FIRSTFARADAY
Melvin Brown	Smith Institute
Dr Tim Boxer	Smith Institute

Smith Institute

The **Smith Institute** manages the Faraday Partnership for Industrial Mathematics and is the leading intermediate organization in the UK coupling industry and academia in the key enabling disciplines of mathematics and computing. The Institute promotes industrial competitiveness through improved collaboration between industry and the science base for the purposes of research, development and technology transfer. The Smith Institute delivers solutions and technical services to companies, through the application of mathematical modelling and analysis. In a knowledge-driven economy, these skills provide cost-effective solutions to operational or design problems, and are also vital to the formulation of industrial strategy. The Institute's staff has wide expertise in modelling, data analysis, project management and research coordination.

Website: www.smithinst.co.uk

FIRSTFARADAY Partnership

FIRSTFARADAY (the Faraday Partnership for Innovative Remediation Science and Technology) is a UK Centre of Excellence for Remediation of the Polluted Environment. The core members of FIRSTFARADAY comprise seven academic institutions, four Research and Technology Organisations (RTOs) and The Environment Agency of England and Wales. There is a growing membership of over 200 industrial concerns from SMEs to large companies and from technology providers, problem holders and consultants. The academic partners of FIRSTFARADAY have a range of complementary skill sets and expertise covering civil and chemical engineering, hydrology, geochemistry, microbiology and molecular biology.

The mission of FIRSTFARADAY is

- to develop world-class scientific methods, technologies and tools for the assessment, remediation and management of contaminated land
- to form a dedicated network of academic, industrial and other stakeholders and regulators committed to cost-effective research, technology transfer and training
- to enhance the position of the UK contaminated land and water sector in the global market place

Website: www.firstfaraday.com