MODELLING AND SIMULATION FRAMEWORK FOR REACTIVE TRANSPORT OF ORGANIC CONTAMINANTS IN BED-SEDIMENTS USING A PURE JAVA OBJECT-ORIENTED PARADIGM

JASON GO JULIA STEGEMANN

Department of Civil and Environmental Engineering
Chadwick Bldg., UCL
Gower St., London
WC1E 6BT
UK
Email: ucesjgo@ucl.ac.uk
Email: j.stegemann@ucl.ac.uk

GRAHAM ROBERTS

Department of Computer Science
Malet Place, Engineering Bldg., UCL
Gower St., London
WC1E 6BT
Email: g.roberts@cs.ucl.ac.uk

IAN ALLAN

School of Biological Sciences
University of Portsmouth
Portsmouth, PO1 2DY
UK
Email:
Ian.Allan@port.ac.uk

ABSTRACT

Numerical modelling and simulation of organic contaminant reactive transport in the environment is being increasingly relied upon for a wide range of tasks associated with risk-based decision-making, such as prediction of contaminant profiles, optimisation of remediation methods, and monitoring of changes resulting from an implemented remediation scheme. The lack of integration of multiple mechanistic models to a single modelling framework, however, has prevented the field of reactive transport modelling in bed-sediments from developing a cohesive understanding of contaminant fate and behaviour in the aquatic sediment environment. This paper will investigate the problems involved in the model integration process, discuss modelling and software development approaches, and present preliminary results from use of CORETRANS, a predictive modelling framework that simulates 1-dimensional organic contaminant reaction and transport in bed-sediments.

KEYWORDS: reactive transport modelling, integrated modelling framework, organic contaminants.

INTRODUCTION

Reactive transport modelling is a valuable tool in understanding the fate and transport of contaminants in bed-sediments. Developed and mature models have been used for the analysis of datasets, from bench-scale laboratory set-ups to field-scale demonstrations, to interpret complex interactions between processes occurring in the subsurface systems (e.g., Boudreau, Meysman, & Middelburg 2004; Meysman et al. 2003b; Thibodeaux, Valsaraj, & Reible 2001). Simulations of various phenomenological observations from reactive transport studies in aquatic bed-sediments have gradually developed fundamental principles in sediment biogeochemistry. Results of these simulation studies have even been used as key components in public policy debates and likewise been considered for regulatory purposes (Steefel & Van Cappellen 1998; Tunkel et al. 2005).

The field of reactive transport modelling over the past quarter century has dynamically evolved from facile analytical models with over-simplified assumptions to realistic and complex numerical representations of the intricate array of interactions within the sediment environment (e.g., Allan et al. 2005; Boudreau 1997; Daniels et al. 1998; Meysman, Middelburg, Herman, & Heip 2003b; Soetaert, Herman, & Middelburg 1996). Moreover, with the significant increase in computational power and capability, reactive transport codes can now potentially accommodate complex phenomena (e.g., nonlinear behaviour arising from wide temporal and spatial variations) previously unaccounted for in legacy models. For example, the diffusive transport of organic contaminants has evidently progressed from a simple Fickian process to a spatially explicit transport mechanism affected by sediment geometrical and organic matter content heterogeneity (e.g., Chiou et al. 2000; Kleineidam, Schüth, & Grathwohl 2002; LeBouef & Weber Jr. 1997; Weber, McGinley, & Katz 1992; Xia & Pignatello 2001). The presence of a diverse benthic community and its impact to the fate and transport of organic contaminants in bed-sediments have been investigated as well (e.g., Aller 1980; Meysman, Boudreau, & Middelburg 2003; Reible et al. 1996; Thibodeaux, Valsaraj, & Reible 2001). The significant growth in the reactive transport modelling field and the increasing complexity in model developments necessitate data and knowledge integration towards a vital and more cohesive understanding of contaminant fate and behaviour in bed-sediments.

With the recognition of the risks posed by contaminated sediments to both the environment and human health (See, for example, Calmano, Ahlf, & Forstner 1996; Jönsson et al. 2003; Lange et al. 1998; Warren et al. 2003) and the necessity for compliance with the recent European Water Framework Directive (2000/60EC), an improved quantitative understanding of the various processes governing sediment biogeochemistry therefore needs to be elucidated and contaminant distribution must be ascertained. Thus, the main challenge of this research is the development of an integrated predictive model that serves as a framework to simulate and evaluate current mechanistic models that best describe the reactive transport of organic contaminants in bed-sediments under site-specific conditions and identify knowledge gaps. In this paper, we will investigate the issues underpinning the process of developing modelling frameworks; discuss modelling and software development approaches; and present CORETRANS, an integrated model framework for modelling and simulating organic contaminant reaction and transport in bed-sediments, in its initial stages.

ISSUES IN REACTIVE TRANSPORT MODELLING

Software development, regardless of the method computing environment, still follows the traditional order of feasibility assessment, requirement analysis, design formulation, and code implementation (Nguyen 2006). Conventional modelling practice dictates that once the entire problem tasks (i.e., feasibility, requirement, and design) have been analysed and mapped out, translation to a code using a programming language of choice follows. Resulting model codes built using traditional procedural programming, however, tend to have fixed formulations and rigid structures. The subsequent application of these models to simulation scenarios other than that to which they were originally intended will, thus, result to either oversimplifications or diminished predictive capability. Meysman, et. al. (2003a) further pointed out that a lack of transparency in model complexity often limits its application only to those who actually developed the model. Moreover, model sensitivity and uncertainty may be compromised for these complex models (Snowling & Kramer 2001). Thus, various constraints in the modelling process have been identified as follows:

- Scientists and engineers with minimal modelling skills are faced with the daunting task of learning how to build and apply computer models or modify existing codes to suit observed data. If the task proves to be too difficult, building a simpler model –either from electronic spreadsheets or through the use of analytical solutions, becomes the next option. The apparent failure in the transfer of knowledge stems from the lack of an inter-disciplinary data computing management strategy where environmental modellers need not turn into proficient software engineers in order to develop sophisticated environmental models.

- The demand for new numerical techniques increases as more complex phenomena arise in the field of environmental modelling. Integration of newly acquired information from various components of reactive transport phenomena in a single model requires complicated numerical solutions. Temporal and spatially explicit data will also likely require hybrid mathematical techniques, additional output visualisations and extensive computing resources.

- Legacy models (e.g., FORTRAN models), although effectively performing the tasks they were designed for, can not accommodate new modelling requirements resulting from recent discoveries in science. Updating old codes with new features or integrating the model with existing databases and other softwares demands certain degrees of algorithm flexibility and model extensibility. Outdated programming practices (e.g., procedural programming, top-down approach), however, prevent such modifications. The need for a shift in programming paradigm coupled with software quality assurance in terms of design, hence, becomes urgent.

- With the ensuing increase in model complexity, predictions become highly uncertain. Biased prediction processes (i.e., approximation of parameters, subjective interpretation of assumptions), calibration errors, and lack of an integrated uncertainty analysis will greatly impact model prediction accuracy.

INTEGRATED MODELLING FRAMEWORK

Advances in the field of reactive transport modelling in bed-sediments have resulted in the proliferation of numerous models developed using different strategies and coded in various programming languages. Similar trends are experienced in other reactive transport disciplines such as groundwater geological systems, contaminant hydrology and early diagenesis. To address this problem and ease the burden of repetitive model coding, modelling frameworks are adopted (Argent 2004; Reed, Cuddy, & Rizzoli 1999). This innovative architectural system offers the benefits of modularity, where building blocks (e.g., contaminant species, transport process, parameters) are integrated in a systematic and efficient manner to form complex model systems without rewriting the underlying codes and performing subsequent recompilation. The dynamic structure of a modelling framework with its innovative support components can advance the simulation process by providing graphical visualisations and interactive mechanisms. To date, the most efficient tool in constructing these frameworks is the application of the object-oriented (OO) paradigm which offers structural flexibility and robustness, and code reusability and extensibility (Page-Jones 2000; Pressman 2001). Under the OO approach, key model systems are identified as 'objects' with distinct attributes and behaviours. Objects sharing the same characteristics are built using a prototype called 'class' which contains variables and methods. Objects consequently communicate with one another by invoking the inherent methods created within the class. Thus, the resulting model can be simply viewed as a collection of interacting objects.

A wide range of modelling frameworks has been developed for various disciplines in reactive transport modelling. For example, early diagenetic models can be investigated using MEDIA (Meysman, Middelburg, Herman, & Heip 2003b) where elements, species, parameters and reactions are modelled as objects that a user can simply select from a toolbox. Li and Liu (2003) have developed a novel 'digital laboratory' for groundwater research where modellers and students can investigate and visualise groundwater systems. The Interactive Groundwater (IGW) software is equipped with geographic information system (GIS) technology for simulating contaminant transport in the subsurface. Other environmental modelling frameworks such as the Ecological Component Library for Parallel Spatial Simulation (ECLPSS) (Wenderholm 2005), the Java implementation of the Discrete Event System (JDEVS) (Filippi & Bisgambiglia 2004), the Interactive Component Modelling System (ICMS) (Reed, Cuddy, & Rizzoli 1999), the Spatial Modelling Environment (SME) (Voinov et al. 1999), and the Modular Modelling System (MMS) (Leavesley et al. 1996; Leavesley et al. 2002) have been developed to simulate various environmental processes. These modelling frameworks all share the following desirable features:

- a modelling (or *problem-solving*) environment that provides a virtual problem domain equipped with visualisation and advanced numerical solvers designed for model construction where components are selected from a toolbox or built based on existing templates;
- a suite of graphical user interface (GUI)-based simulation control components that facilitates selection of model scenarios and input/output (I/O) data operations employing text editors for code generation and compilation and/or single button click implementation;
- a computing resource package that provides numerical solutions, optimisation procedures, and statistical analyses;
- a database management system for an easy data retrieval process that is interoperable with the simulation process to optimise modelling functionalities; and
- an efficient documentation system for operational use and maintenance purposes.

Following the success of these environmental modelling frameworks, we proposed to develop a discrete and continuous event specification based framework for simulating the reactive transport of organic contaminants in bed-sediments using a pure Java object-oriented approach.

CORETRANS: AN INTEGRATED REACTIVE TRANSPORT MODEL FRAMEWORK IN BED-SEDIMENTS

Model Formulation and Structure

The CORETRANS model is derived as an extensible partial differential equation (equation 1) which governs 1-dimensional reactive transport of a single chemical constituent in bed-sediments given by the mass conservation law of the form:

$$\frac{\partial}{\partial t}\left(C+\frac{\rho}{\varphi}S\right)+\upsilon\frac{\partial C}{\partial x}-\frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)=\sum R_{\sin k/source} \quad (1)$$

where C and S are, respectively, the soluble and absorbed concentrations of the chemical contaminant within the bed-sediment of constant sediment density *ρ*. The sediment porosity *φ* is assumed to be invariant with time *t* (i.e., steady-state compaction). The advective velocity *v*, diffusivity *D*, and additional sink/source *R* (e.g., bioirrigation, deposition, bioturbation) completes the advective-diffusive system that typically describes the vertical migration of the contaminant in the bed-sediment from the sediment-water interface down to the desired depth *x*.

Using the OO approach, the CORETRANS modelling framework is designed as a three-tier, multiple window application package built using the Java 2 Platform Standard Edition (J2SE version 1.4.1). The objects created within the OO system are grouped into three categories of classes – graphical user interface (GUI), problem domain, and the data access classes. The CORETRANS GUI, in its initial stage, provides integrated functionalities for pre-processing of the simulation scenario, such as constructing the reactive transport model, entering data, and displaying graphical and/or tabular representations of simulation outputs. It is continually being developed using the Eclipse 3.0 platform to further include post-simulation processes such as optimisation of key parameters and calibration of the resulting model on the basis of experimental results.

Within the problem domain classes, objects are further separated into contaminants species, reactive transport processes, and simulation parameters. The constitutive laws describing the reactive transport of organic contaminants in bed-sediments are integrated as coupled components users can simply select. This modular structure enables the application users to build their own reactive transport model using single button click implementation and execution. The simulation parameter objects, once instantiated, prompt the user to either choose built-in values via the CORETRANS database or enter their own parametric values. User-defined parametric values are integrated into the problem domain using simple accessor methods (e.g., getSedimentDepth, setSedimentDepth).

Contaminant species are selected using an object-oriented database, where data access classes are invoked to store and retrieve values for the selected contaminant species and their physical and chemical properties. The CORETRANS database is accessed through a set of data access classes employing the Java Database Connectivity (JDBC) protocol and is currently maintained using a remotely hosted MySQL database server (release 4.0.16).

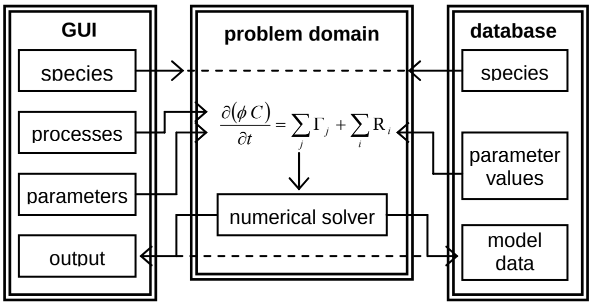


Figure 1: Schematic diagram of CORETRANS three-tier structure

The three-tier structure (see Figure 1) implements client-server architecture where the GUI, problem domain and data access operations may exist in various sites which can make the deployment of the CORETRANS package easier. Further, the classes within each tier are independent of each other allowing them to be easily changed without affecting those in another tier making the entire OO system extensible and easy to maintain.

Numerical Procedure

A numerical solver based on finite element systems also written in Java is integrated in the CORETRANS package to solve and simulate the customised model as a combined discrete and continuous event. The customised model equation is numerically solved using the Method of Lines where the right-hand side of the equation is discretised into finite grids while the time variable remains continuous. The method thus effectively reduces the model equation to a system of ordinary differential equations which can be subsequently solved using any ODE integration procedures (e.g., Runge-Kutta-Fehlberg method) (Schiesser 1991). Boundary conditions such as Dirichlet (concentration), Neumann (flux) and Robin's (mixed conditions) are available as user-defined selections.

Basically, the selected reactive transport processes generate a partial differential equation code that overrides an inherent method within the numerical solver. Java's polymorphic feature (i.e., method overriding) enables CORETRANS to solve multiple equations (e.g., PDEs that describe contaminant porewater and sediment-bound profiles) in a single simulation run.

Java Performance

The increasing complexity in reactive transport models continually drives environmental modellers into using object-oriented technologies. Java, as a pure OO language, offers a suite of desirable features that make it ideal not only for GUI web-centric applications but for developing extensible portable modelling frameworks designed to solve complex problems based on finite element systems as well. Java's numerical computing efficiency relies on the continued development of modern compiler technologies. Sun Microsystem's Just In Time (JIT) compiler, for example, facilitates translation of Java byte-codes to machine code at runtime making it competitive with either C++ or Fortran. Thus, CORETRANS' simulation runs are optimised (e.g., faster iterations, efficient garbage collections) once executed under modern Java Runtime Environments (JREs).

Model Validation and Discussion

For the initial validation of the CORETRANS model, a dataset from a fluvarium channel experiment for the transport and distribution of selected trace level organic contaminants in a riverine environment was modelled, as reported in Allan et. al (2004). The study aimed to understand the various processes that determined the depth distribution of these contaminants. Using Fortran 90, a basic 1-dimensional diffusion-sorption-degradation (DSD) procedural program was built to calculate diffusion-controlled concentration-depth profiles for micro-organic contaminants in the sediment porewater and the whole sediment bed, based on temporal changes in concentration in the overlying water. The numerical approach of the DSD model allows temporally and spatially flexible definition of sediment characteristics and processes. To test the efficacy of the CORETRANS modelling framework, Allan's Fortran 90 - DSD model given in equation 2 was reconstructed and simulated.

$$\frac{\partial C}{\partial t} = \frac{D_e}{1 - \ln\left(\varphi^2\right)} \frac{\partial^2 C}{\partial x^2} - k_{\deg} C \qquad (2)$$

The effective diffusivity D_e was solved using Equation (3):

$$D_e = \frac{D_t}{1 + \frac{\rho}{\varphi} K_d} \qquad (3)$$

where the theoretical diffusivity D_t was approximated using the Wilke-Chang correlation and corrected using a retardation factor incorporating the linear partitioning of the contaminant to the sediment particle matrix. The sediment porosity φ as a function of depth was modelled using a power law equation. An optimised first-order degradation constant (k_{deg}) completed the set of parameters for the DSD model simulation. Three simulation scenarios were run for the DSD model using CORETRANS: (1) use of a single optimised K_{OM} for the linear partitioning sorption mechanism (i.e., $k_d = K_{OM}\ f_{OM}$) with no degradation term; (2) use of a distribution coefficient k_d as a function of depth modelled using a power law equation, still with no degradation term, and; (3) use of power function distribution coefficient k_d with a single degradation term. The parameters utilised in the simulation process are summarised in Tables 1 and 2.

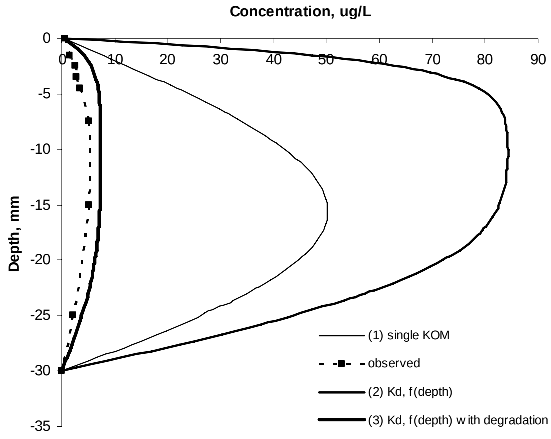
Table 1: Simulation parameters for the DSD model

Parameters	Values
Sediment depth, x, *mm*	30
Number of layers	100
Simulation time, *weeks*	6
Initial concentration, C_o, $\mu g\ L^{-1}$	84.6
Concentration, C at x_o, $\mu g\ L^{-1}$	0.54
Concentration, C at x, $\mu g\ L^{-1}$	0

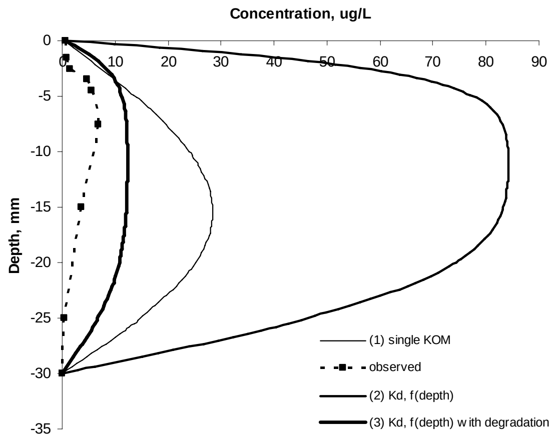
Table 2: Environmental parameters for the DSD model

Parameters	Channel 1	Channel 2
Sediment density, $kg\ L^{-1}$	2.50	2.50
Temperature, *K*	288	288
Organic matter content, f_{OM}	0.08	0.08
K_{OM}, $L\ kg^{-1}$	23	12
K_d, *f*(depth, mm) = a x (depth)$^{-b}$		
a	180.94	130.39
b	1.14	0.99
k_{deg}, sec^{-1}	6.72 x10^{-7}	5.31 x10^{-7}
φ, *f*(depth, mm) = a x (depth)$^{-b}$		
a	0.69	0.69
b	0.12	0.12

Porewater concentration-depth profiles of the organic contaminant lindane from the experimental dataset under dark conditions were compared to the predicted profiles generated from the CORETRANS model as shown in Figure 2.



(a) channel 1



(b) channel 2

Figure 2: Concentration-depth profiles for lindane under dark conditions for both channels. Data from (Allan et al. 2004)

The original Fortran 90 package used for the DSD model required three different program codes for the compilation and execution of all simulation scenarios. The CORETRANS framework, however, made it much simpler to investigate behavioural methods from the simulation process. The following observations demonstrate the effectiveness of CORETRANS as a tool in simulating reactive transport models in bed-sediments:

- The DSD model can easily be simulated as CORETRANS has all the typical constitutive reactive transport laws (i.e., diffusion, sorption and degradation) integrated as GUI-based components (e.g., buttons), which the user can simply select to customise the model.
- Environmental parameters are obtained from the user in a straightforward manner (i.e., data input in text boxes or single button click implementation). Java’s effective encapsulation system hides the internal structure of the objects used in the framework thereby protecting the modelling

framework from corruption due to model re-codification.

- Graphical and/or tabular outputs from the simulation are easily displayed.

From the simulation exercises, it is apparent that the sorption and degradation mechanisms considered in the model are significant processes in the analysis of the vertical migration and distribution of the contaminant in bed-sediments. The various sorption isotherms used in the simulation process significantly affected the goodness of fit of the predicted profiles. Nonlinear isotherms and their various combinations as well as other reactive transport processes are yet to be tested and might show a further improvement in fit. Clearly, the ease in constructing reactive transport models using the CORETRANS framework without the burden of coding enables modellers to concentrate on identifying knowledge gaps in the field of reactive transport in bed-sediments.

ONGOING AND FUTURE WORKS

The field of reactive transport modelling is continuously evolving. Various research groups on the distribution of hydrophobic organic contaminants in natural bed-sediments have significantly contributed to the pool of knowledge collected over the years. Developing simulation tools for reactive transport modelling, however, can be tedious especially to scientists without good programming skills. Thus, CORETRANS aims to provide a general modelling framework for evaluating current models and identifying knowledge gaps concerning contaminant reaction and transport in bed-sediments.

As demonstrated, CORETRANS can presently simulate various reactive transport processes from a set of pre-simulation control components. Future work will focus on the development of post-simulation components such as: (1) statistical analyses for calibration of customised models; (2) optimisation procedures for selected environmental parameters, and; (3) a numerical sensitivity analysis component in order to understand the significance of each process, parameter and variable in the overall system, and the extent of their effects under realistic conditions. Further verification and validation will be done as each post-simulation component is integrated into CORETRANS.

REFERENCES

Allan, I. J., House, W. A., Parker, A., & Carter, J. E. 2004, "Transport and distribution of lindane and simazine in a riverine environment: measurements in bed sediments and modelling", *Pesticide Management Science*, vol. 60, no. 5, pp. 417-433.

Allan, I. J., House, W. A., Parker, A., & Carter, J. E. 2005, "Diffusion of the Synthetic Pyrethroid Permethrin into Bed-Sediments ", *Environmental Science and Technology*, vol. **39**, no. 2, pp. 523-530.

Aller, R. C. 1980, "Quantifying solute distributions in the bioturbated zone of marine sediments by defining an average microenvironment.", *Geochimica et Cosmochimica Acta*, vol. 44, pp. 1955-1965.

Argent, R. M. 2004, "An overview of model integration for environmental applications--components, frameworks and semantics", *Environmental Modelling & Software*, vol. 19, no. 3, pp. 219-234.

Boudreau, B. P. 1997, "A one-dimensional model for bed-boundary layer particle exchange", *Journal of Marine Systems*, vol. 11, no. 3-4, pp. 279-303.

Boudreau, B. P., Meysman, F. J. R., & Middelburg, J. J. 2004, "Multicomponent ionic diffusion in porewaters: Coulombic effects revisited", *Earth and Planetary Science Letters*, vol. 222, no. 2, pp. 653-666.

Calmano, W., Ahlf, W., & Forstner, U. 1996, "Sediment quality assessment: chemical and biological approaches," in *Sediments and Toxic Substances: Environmental Effects and Toxicity*, W. Calmano & U. Forstner, eds., Springer, Germany, pp. 1-29.

Chiou, C. T., Kile, D. E., Rutherford, D. W., Sheng, G., & Boyd, S. A. 2000, "Sorption of Selected Organic Compounds from Water to a Peat Soil and Its Humic-Acid and Humin Fractions: Potential Sources of the Sorption Nonlinearity", *Environmental Science and Technology*, vol. 34, no. 7, pp. 1254-1258.

Daniels, W. M., House, W. A., Zhmud, B. V., Rae, J. E., & Parker, A. 1998, "Diffusive movement of simazine and lindane in river-bed sediments", *Pest Management Science*, vol. 54, no. 3, pp. 212-222.

Filippi, J. B. & Bisgambiglia, P. 2004, "JDEVS: an implementation of a DEVS based formal framework for environmental modelling", *Environmental Modelling & Software*, vol. 19, no. 3, pp. 261-274.

Jönsson, A., Gustafsson, Ö., Axelman, J., & Sundberg, H. 2003, "Global Accounting of PCBs in the Continental Shelf Sediments", *Environmental Science and Technology*, vol. **37**, no. 2, pp. 245-255.

Kleineidam, S. E., Schüth, C., & Grathwohl, P. 2002, "Solubility-Normalized Combined Adsorption-Partitioning Sorption Isotherms for Organic Pollutants", *Environmental Science and Technology*, vol. 36, no. 21, pp. 4689-4697.

Lange, R., Hutchinson, T. H., Scholz, N., & Solbe, J. 1998, "Analysis of the ECETOC aquatic toxicity (EAT) database - II - comparison of acute to chronic ratios for various aquatic organisms and chemical substances.", *Chemosphere*, vol. 36, pp. 115-127.

Leavesley, G. H., Markstrom, S. L., Brewer, M. S., & Viger, R. J. 1996, "The modular modeling system (MMS) – The physical process modeling component of a database-centered decision support system for water and power management", *Water, Air, & Soil Pollution (Historical Archive)*, vol. 90, no. 1 - 2, pp. 303-311.

Leavesley, G. H., Markstrom, S. L., Restrepo, P. J., & Viger, R. J. 2002, "A modular approach to addressing model design, scale, and parameter estimation issues in distributed hydrological modelling", *Hydrological Processes*, vol. 16, no. 2, pp. 173-187.

LeBouef, E. J. & Weber Jr., W. J. 1997, "A Distributed Reactivity Model for Sorption by Soils and Sediments. 8. Sorbent Organic Domains: Discovery of a Humic Acid Glass Transition and an Argument for a Polymer-Based Model", *Environmental Science and Technology*, vol. 31, no. 6, pp. 1697-1702.

Li, S.-G. & Liu, Q. 2003, "Interactive Groundwater (IGW): An innovative digital laboratory for groundwater education and research", *Computer Applications in Engineering Education*, vol. 11, no. 4, pp. 179-202.

Meysman, F. J. R., Boudreau, B. P., & Middelburg, J. J. 2003, "Relations Between Local, Nonlocal, Discrete and Continuous Models of Bioturbation", *Journal of Marine Research*, vol. 61, pp. 391-410.

Meysman, F. J. R., Middelburg, J. J., Herman, P. M. J., & Heip, C. H. R. 2003a, "Reactive transport in surface sediments. I. Model complexity and software quality", *Computers & Geosciences*, vol. 29, no. 3, pp. 291-300.

Meysman, F. J. R., Middelburg, J. J., Herman, P. M. J., & Heip, C. H. R. 2003b, "Reactive transport in surface sediments. II. Media: an object-oriented problem-solving environment for early diagenesis", *Computers & Geosciences*, vol. 29, no. 3, pp. 301-318.

Nguyen, T. N. 2006, "A decision model for managing software development projects", *Information & Management*, vol. 43, no. 1, pp. 63-75.

Page-Jones, M. 2000, *Fundamentals of Object-Oriented Design in UML* Dorset House Publishing, New York, NY.

Pressman, R. S. 2001, *Software Engineering: A Practitioner's Approach* McGraw Hill, New York.

Reed, M., Cuddy, S. M., & Rizzoli, A. E. 1999, "A framework for modelling multiple resource management issues--an open modelling approach", *Environmental Modelling and Software*, vol. 14, no. 6, pp. 503-509.

Reible, D. D., Popov, V., Valsaraj, K. T., Thibodeaux, L. J., Lin, F., Dikshit, M., Todaro, M. A., & Fleeger, J. W. 1996, "Contaminant fluxes from sediment due to tubificid oligochaete bioturbation", *Water Research*, vol. 30, no. 3, pp. 704-714.

Schiesser, W. E. 1991, *The Numerical Method of Lines: Integration of Partial Differential Equations* Academic Press, San Diego, CA.

Snowling, S. D. & Kramer, J. R. 2001, "Evaluating modelling uncertainty for model selection", *Ecological Modelling*, vol. 138, no. 1-3, pp. 17-30.

Soetaert, K., Herman, P. M. J., & Middelburg, J. J. 1996, "A model of early diagenetic processes from the shelf to abyssal depths", *Geochimica et Cosmochimica Acta*, vol. 60, no. 6, pp. 1019-1040.

Steefel, C. I. & Van Cappellen, P. 1998, "Reactive transport modeling of natural systems - Preface", *Journal of Hydrology*, vol. 209, no. 1-4, pp. 1-7.

Thibodeaux, L. J., Valsaraj, K. T., & Reible, D. D. 2001, "Bioturbation-Driven Transport of Hydrophobic Organic Contaminants from Bed Sediment", *Environmental Engineering Science*, vol. 18, no. 4, pp. 215-223.

Tunkel, J., Mayo, K., Austin, C., Hickerson, A., & Howard, P. 2005, "Practical considerations on the use of predictive models for regulatory purposes", *Environmental Science and Technology*, vol. 39, no. 7, pp. 2188-2199.

Voinov, A., Costanza, R., Wainger, L., Boumans, R., Villa, F., Maxwell, T., & Voinov, H. 1999, "Patuxent landscape model: integrated ecological economic modeling of a watershed", *Environmental Modelling and Software*, vol. 14, no. 5, pp. 473-491.

Warren, N., Allan, I. J., Carter, J. E., House, W. A., & Parker, A. 2003, "Pesticides and other micro-organic contaminants in freshwater sedimentary environments--a review", *Applied Geochemistry*, vol. 18, no. 2, pp. 159-194.

Weber, W. J., McGinley, P. M., & Katz, L. E. 1992, "A distributed reactivity model for sorption by soils and sediments. 1. Conceptual basis and equilibrium assessments", *Environmental Science and Technology*, vol. 26, no. 10, pp. 1955-1962.

Wenderholm, E. 2005, "Eclpss: a Java-based framework for parallel ecosystem simulation and modeling", *Environmental Modelling & Software*, vol. 20, no. 9, pp. 1081-1100.

Xia, G. & Pignatello, J. P. 2001, "Detailed Sorption Isotherms of Polar and Apolar Compounds in a High-Organic Soil", *Environmental Science and Technology*, vol. 35, no. 1, pp. 84-94.

AUTHOR BIOGRAPHIES

JASON V. GO is a PhD student in the Department of Civil and Environmental Engineering at UCL. He has obtained his MS degree in Environmental Engineering from the University of the Philippines in 2003.

JULIA A. STEGEMANN is a senior lecturer in the Department of Civil and Environmental Engineering at UCL. She has been doing research in treatment, characterisation and leaching of industrial wastes for more than twenty years. With Bachelor's and Master's degrees in chemical engineering, and a PhD in environmental engineering, she has experience in laboratory development of technologies and test methods, preparation of regulatory guidance documents, implementation and evaluation of technologies at field scale and computer modelling.

GRAHAM ROBERTS is a lecturer in the Department of Computer Science at UCL. He obtained his PhD from Queen Mary College, University of London in the area of type systems for object-oriented languages. His research covers the areas of object-oriented programming, testing, agile development and the model driven architecture (MDA).

IAN J. ALLAN a researcher in the School of Biological Sciences at the University of Portsmouth. He obtained his PhD from the Postgraduate Research Institute for Sedimentology at the University of Reading in 2002 in collaboration with the Centre for Ecology and Hydrology Dorset. After one year spent working on contaminated soils at the University of East Anglia, he is working on the testing of tools for water quality monitoring (SWIFT-WFD project).

MOBILE HEALTHCARE NETWORK: A SIMULATION APPROACH TO SYSTEM DESIGN

KHAMISH MALHOTRA, STEPHEN GARDNER

School of Electronics
University of Glamorgan
Pontypridd, CF37 1DL, Wales, UK
E-mail: kmalhotr,sgardner@glam.ac.uk

ABSTRACT

This paper describes investigations into the implementation of different software tools to simulate the behaviour of GPRS traffic and its utilisation for the performance analysis of healthcare wireless applications. The theme of this paper surrounds the issues concerning the simulation and modelling of GPRS networks for remote monitoring applications. Different tools have been explored and the eventual outcome was to utilise NS2 (Network Simulator) to achieve the research results. The focus of the work is centred on the evaluation of a model of a healthcare mobile network, in real-time, through the analysis of results from validated simulation exercises.

KEYWORDS: Wireless Telemedicine, Secure wireless networks, Simulation Modelling, Remote Patient monitoring applications, Performance Evaluation, NS2

INTRODUCTION

Developing a simulation platform to specifically study patient support in mobile networks was a fundamental requirement of the overall research programme being undertaken. Under question is how healthcare applications will behave over GPRS with the added requirement of various security mechanisms. Remote patient monitoring systems are characterised by especially sensitive requirements relating to safety, security, accuracy, reliability, and adaptability.

Over recent years, various remote monitoring applications have been proposed [1, 2], but little information about the effects of security exposures in terms of network performance has been available. This research programme identifies security issues, that are specific to healthcare sector, and the simulations will allow a variety of quality of service and performance issues to be investigated.

A real-time implementation, the system is also being built and test results used to validate the simulation. Some of the modelling tools required include mathematical techniques from queuing theory, Markov models, probabilistic models and Petri-net models. The simulation environment was also an important criterion, as specific and specialist modules are required for the research that do not currently exist. The need to be able to implement the mathematical models developed, using a relatively straightforward programming interface and language was also imperative. This paper highlights part of the ongoing research [4] where a test-bed has been created integrating Linux based embedded system to a server via a Mobile (GPRS) channel for remote patient monitoring and alarm applications.

The performance characteristics of commercially available mobile channels must be addressed before integrated mobile Internet services can be commercially deployed in the healthcare sector. The contemporary approach of this work is to provide modelling of secure network parameters and processes. Performance of the system is more important when a time critical application of patient’s health is taken into account. Security is a serious concern in healthcare mobile system as the wireless medium is open for public access. The factors affecting secure mobile systems are as follows:

Confidentiality: The property that information is not made available to unauthorized individuals or processes.

Authentication: This requires the parties in a transaction to provide a means of proving their true identity. In wireless data realms this is provided by a means of trusted identification.

Integrity: This insures the detection of any change in the contents of a transaction. For a digital domain, integrity is guaranteed by analyzing transmission contents at reception and using algorithms which determine if the contents have been altered. In addition a digital signature may be used to provide a stronger test for integrity.

Non-repudiation: It demands that a party to a transaction cannot falsely claim that they did not participate in that transaction.

Complete security demands that the three entities in a network i.e. software, hardware and data must be secure. In case of remote patient monitoring the security needs to be implemented at both the mobile side and at the Internet medium.