Program 2: Hydrodynamics and Modelling of Complex Groundwater Systems
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Numerical models form a vital and increasingly important component of modern quantitative hydrogeology; they are both a fundamental way of investigating complex groundwater hydrodynamics and an invaluable tool in the formulation of research questions and hypotheses. It is widely understood that as the sophistication of hydrogeologic conceptual models evolves major research challenges will be encountered on at least two levels: (a) the conceptual understanding of the inherent physics, chemistry and groundwater dynamics associated with these problems, and (b) the incorporation and simulation of increasingly complex groundwater processes in the numerical simulators used to understand them. A number of significant complex groundwater processes will be examined in this program using modelling as the investigative tool. *Key investigators: CI Simmons, CI Werner and PI Cook, with assistance from CI Lockington, CI Li and CI Kelly.*

Sub-program 2A: Uncertainty in groundwater flow estimation. Estimating groundwater flow rates in heterogeneous aquifers remains a critical challenge for modern quantitative hydrogeology. Commonly-used approaches rely on hydraulic methods (e.g. pump tests) as a basis for using Darcy's Law, or environmental tracers (e.g. CFC's, ^{14}C and ^{3}H) for estimating groundwater age. Previous studies have assessed uncertainty separately in these approaches (de Marsily, 2005). This Sub-program is, however, the first systematic and unified theoretical assessment of the two approaches. Hydraulic and tracer approaches will be simulated in a heterogeneous system. Both heterogeneous sedimentary aquifers with appropriate geostatistical properties (mean, standard deviation, correlation length scales) and fractured rock aquifers with appropriate discrete fracture properties derived from statistical distributions (fracture length, aperture, separation, connectedness) will be considered. The Sub-program is cutting-edge in that it will attack the fundamental research questions (i) how uncertainty in flow rate estimation is linked to degree and structure of heterogeneity, and (ii) which method will have the lowest uncertainty in a particular system. Quantifying uncertainty in groundwater flow estimation is a very significant unresolved problem in groundwater hydrology.

Sub-program 2B: Heterogeneity in groundwater fluids and geologic structures. In certain hydrogeologic situations, groundwater fluid properties (such as density and viscosity) vary because of changes in solute concentration, temperature and pressure of the groundwater. These spatiotemporal variations in groundwater fluid properties can have critical consequences for groundwater flow and solute transport. Previous studies (Simmons, 2005) have identified that the prediction of dense plume migration rates and pathways is extremely complex and in heterogeneous geologic systems is currently not possible. This work will test the hypothesis that 'microscopic indicators' of dense plume migration (e.g. number of unstable fingers) may not be amenable to prediction but that 'macroscopic indicators' (e.g. salt flux rates or centre of mass) may be. We contend that an equivalent homogeneous but anisotropic system coupled with macroscopic indicators can be used to provide reliable predictions for dense plume migration in certain heterogeneous systems. We use numerical models and a combined geostatistical-Monte Carlo framework to explore this hypothesis. This Sub-program will provide new fundamental understanding about upscaling groundwater processes in systems where both heterogeneous groundwater fluids and heterogeneous geologic structures control groundwater flow and solute transport processes.

Sub-program 2C: Highly transient, spatially-distributed surface water–groundwater interaction. Models of surface–groundwater interaction commonly assume steady state conditions in time and homogeneity of river bed conductance in space. These conditions are rarely true in real hydrogeologic systems. Surface water systems are often highly dynamic and they are spatially-distributed features in the landscape. In addition, riverbed conductance, a vital control on surface water – groundwater interaction, is known to vary by 6-7 orders of magnitude (Calver, 2001). Current modelling approaches for surface water-groundwater interaction usually require surface water features to be specified *a priori* as simple boundary conditions that are fixed in space and time. In ephemeral systems, however, the presence of surface water bodies is highly time dependent. The generation and persistence of surface water features will be a function of geologic, geomorphologic and climatic controls. There is a complex but poorly understood interplay between surface water and groundwater processes that lead to the spatially–distributed formation, and transient persistence, of surface water features and hence surface water – groundwater interactions. These processes are extremely oversimplified in current modelling approaches. This Sub-program will utilise powerful numerical models to simulate the evolution and dissipation of highly dynamic and spatially–distributed surface water features and hence surface water – groundwater interactions. We will employ state of the art fully-coupled models such as HydroGeoSphere (Therrien et al., 2005) to simulate three dimensional explicit surface flow, vadose zone, and groundwater flow processes. Models will be constrained using hydraulic and tracer data, including heat. This advanced form of highly coupled, explicit, surface water – groundwater interaction modelling is one of the most fundamental next advances required for computational simulation in this field of hydrogeology.

Sub-program 2D: Simplicity versus complexity in groundwater modelling. This Sub-program is driven by an urgent need to build better practical, complex, regional groundwater models that can be used with greater confidence in solving water management questions. It is founded on the well-accepted premise that hydrogeology is *model rich* and *data poor*. The predictive value of groundwater models is often recognised to be poor, in large part due to our inherent inability to characterise critical hydrogeologic parameters at the requisite spatial and temporal scales and form the appropriate conceptual models (Bredehoeft, 2005). Model calibration is also highly sensitive to recharge rates and hydraulic conductivities. If both are ill-constrained, a calibrated model may be of little, if any, predictive value. This research will develop techniques and methods to significantly improve the predictive value of models. The spatiotemporal pattern of evapotranspiration and recharge may be reliably estimated by upscaling point ground-based measurements using both airborne and spaceborne remote sensing data. Spatially distributed hydraulic conductivity and geologic data from 3D geological models developed in Program 1 will also form a vital basis for improved groundwater flow simulation. Examples of the use of spatially distributed data in hydraulic modelling (Becker, 2006; Brunner et al, 2007) have highlighted major challenges in calibration, parameter uncertainty, optimisation and methods for interpolating/ extrapolating point data in 3D. These challenges will be addressed in this Sub-program. We will also conduct urgently required rigorous quantitative assessments of model parsimony as well as quantifying the trade-offs between model complexity, predictive ability and data acquisition costs. These relationships are rarely, if ever, quantified but are urgently required if we are to maximise the power and usefulness of groundwater modelling.