1. Aims of the collaborative project

We aim to establish collaborations between the Complex Fluids Group at Princeton and the Oxford Centre for Industrial and Applied Mathematics (OCIAM) in the broad spectrum of overlapping research interests in complex fluid flows. This initiative will involve exchange of personnel, as well as organizing and running problem-solving workshops which will unite researchers from both groups to tackle topical issues arising in the real world. Our initial focus will be on the removal of heavy metals from water (see section 3a), although we envisage discussions broadening to include other key problems (see section 3b) over the course of the two years.

2. Personnel

The Princeton Complex Fluids Research Group marries experimental research with theoretical models for a broad spectrum of fluid-dynamical systems with strong interests in physicochemical hydrodynamics. They use experiments, simulations, and modelling to quantitatively characterize problems and to explore new research directions. The group has current projects in microfluidics, wetting of liquids into porous media, splashing dynamics, swelling of soft materials, shear-induced diffusion, water pollution and treatment, and colloidal structuring at interfaces. Some of their research has been motivated (and sponsored) by industrial applications of home and personal care products, oil-field services, fiber coating, float-glass manufacturing, and medical/clinical applications.

The Princeton PI is Prof. Howard Stone (HAS), who leads the Complex Fluids Group. Various members of his research group, which comprises 1 faculty, 8 postdocs, 6 research students, 2 undergraduates, and at any given time 2-6 short term researchers/visitors, will be involved as the projects evolve.

Oxford has a group of mathematical modellers with particular interest in problems arising in the real world, especially those involving fluid mechanics and physicochemical hydrodynamics. The group uses a mixture of modelling, asymptotic analysis and simulation in order to help explain physical phenomena. Current relevant projects involve the modelling and simulation of screen-printing for solar panels, polymer-surfactant mixtures, the adsorption of ionic surfactant, micellar breakdown kinetics, tearfilm dynamics and the formation of multilayer structures at interfaces. These projects all involve collaboration with scientists from other disciplines or with industry.

The Oxford PI is Dr Peter Howell (PDH), Deputy Director of the Oxford Centre for Industrial and Applied Mathematics and an expert in the application of perturbation methods to fluid dynamics. The other key team members are Dr Chris Breward (CJWB) (surfactant flows, thin films) and postdoctoral research associate Dr Ian Griffiths (IMG) (surfactant systems, low-Reynolds-number flows). Dr Dominic Vella (DV) (surface tension phenomena, flow in porous media) will be joining us as a new faculty member from 1 Jan 2011. The wider team at Oxford comprises 9 faculty, 4 postdocs and 5 research students.
The combined team will play a key role in developing a strong network between Oxford and Princeton research staff and students, initiating links that will lead to long-term collaborations.

3. Research activities
We have identified several problems in physicochemical hydrodynamics that will motivate new projects at the intersection of strengths of the Oxford and Princeton groups. The projects are timely and of great social significance.

(a) Removal of heavy metals from water
Arsenic contamination in natural water is a worldwide problem with particular relevance to the developing world. Many other heavy metals are also found in groundwater and pose similar threats to human health. These problems demand the attention of the science and engineering communities because of the significant health issues that are engendered. Dangerous heavy metals such as arsenic, cadmium and nickel generally exist as ions in solution or small nanometre-size particles.

Any remediation or separation strategies must allow for a continuous flow, as occurs in standard filter or water-cleaning processes, and recognize the unique chemical and transport dynamics relevant to these nanoscale, particulate and ion-surface interactions. Despite its importance, this area is lacking in any detailed mathematical analysis, with current approaches heavily reliant on experimental observations and empirical ideas. As a result, the removal of heavy metals from water is ripe for mathematical study, which should lead to new, experimentally testable, hypotheses and approaches.

Several techniques are used currently in the removal of heavy metals from water: coagulation and flocculation, adsorption and ion exchange, membrane filtration, and precipitation. Below we discuss each strategy, the mathematical approaches that we will use to understand these processes, and the expertise upon which we will draw.

(i) Coagulation and flocculation: In the arsenic removal process, coagulation and flocculation are among the most common methods employed [1]. In the coagulation process, a chemical that neutralizes the repulsive forces between colloids is added to the water to facilitate the formation of colloidal aggregates. Once in aggregate form, the particulates may easily be removed from the water. The flocculation process uses a similar approach, with polymers added to solution to form bridging bonds between the arsenic molecules and so form aggregates.

Analogous physicochemical processes are a focus of current research for the proposed research team. In particular, PDH, CJWB and IMG have developed mathematical models to describe the formation and breakdown of aggregates in polymer/surfactant solutions [2]. HAS has experience related to reaction-diffusion problems [3]. We will utilize such models as a basis for the analysis of the coagulation and flocculation processes. In particular, we will consider aggregation kinetic models such as the Becker-Döring equations and exploit the favourability of particular sizes of aggregates to develop reduced models for the system.

(ii) Adsorption and ion exchange: In the adsorption process, contaminated water is passed over a solid bed, typically activated carbon, onto which arsenic is adsorbed and thus removed from the water. The adsorption process occurs mainly due to van der Waals and electrostatic forces between adsorbate and adsorbing surface. Most
studies in this area are empirical in nature, focusing on the type of adsorbent media and the economics of their regeneration [1]. In the ion-exchange process, the arsenic-containing water is passed through an ion-exchange resin loaded typically with chloride ions. The arsenic exchanges for the chloride ions, producing water with a reduced arsenic composition in favour of an increase in chloride concentration.

Nanocrystalline magnetite is a particularly effective adsorbate in removing arsenic from solution, and the effectiveness of the separation of nanometer size magnetite particles from solution is dependent on particle size. [4] write when presenting these data in their highly cited article in Science: “The curves presented are complex polynomials meant to guide the display and are not reflective of any physical model.” The timeliness and need for mathematical modelling could not be clearer.

Again, modelling relevant to such adsorption and ion-exchange dynamics is an area of research expertise for the team. We will extend the models developed by IMG, PDH and CJWB [5] for the adsorption of ionic surfactant at an interface to describe the arsenic removal process and investigate the optimal material properties for adsorption. HAS brings relevant expertise in flow and dispersion in colloidal materials [6]. DV has studied a number of problems involving flow in porous media. Competition with other anions in the contaminated water, such as sulphate ions, can reduce the effectiveness of this process and the results of our mathematical analysis will be used to quantify the impact of such effects.

(iii) Membrane filtration: Nanofiltration and reverse osmosis provide a method to meet regulations for lowered arsenic concentrations in drinking water [7]. Separation of arsenic from the water occurs via a combination of size- and charge-exclusion and preferential passage of more mobile ions. This technology is particularly effective when the intention is to remove more than one chemical.

(b) Relevance to further environmental fluid dynamical issues
External influences, for example electric fields, can be used for the bioremediation in soils (and other porous materials) and the transport of suspensions. Two natural areas for further study with important environmental impact are:

(i) Taylor jetting and tip streaming in the presence of an electric field: When a non-uniform electric field is applied to a thin fluid film it is observed to propagate via capillary spreading and electrostatic forces. The liquid can also be induced to emit thin fluid jets from conical tip structures (Taylor cones) which is known as tip streaming. The behaviour of the fluid propagation and the frequency and volume of fluid emitted in each jet depend on the fluid properties and electric field. We will develop mathematical models to describe the results of experiments on Taylor-cone formation, jet emission and break-up that occur during electrohydrodynamic tip streaming from a liquid film. (Collaborators, Dr P. Kim.)

(ii) Shear enhanced dispersion in suspension flows: When a concentrated Newtonian suspension of neutrally buoyant monodisperse spherical particles flows through a pipe, non-uniformities in concentration are generated through interactions between particles. Of particular interest is the form of the fully developed particle velocity and concentration profiles. Analyzing the influence of shear-enhanced diffusion in the imbibition of a liquid suspension in an air-filled tube will allow us to understand the physically observed increase in concentration of particles at the meniscus, which can lead to clogging, often with catastrophic consequences. (Collaborators, Dr J.)
4. Summary
The modelling described in this proposal will utilize basic approaches to physicochemical hydrodynamics that have been applied successfully to a wide variety of complex problems of colloid science, including transport processes in porous materials. The models to be developed for the problem of heavy metal removal will allow separation processes to be tailored to specific requirements and to minimize the potential treatment costs. It is only with such mathematical modeling that an improved understanding of the separation processes can be established, and new strategies rationally developed. The Oxford-Princeton team combines a range of expertise relevant for tackling this complex problem.

While focusing initially on a specific research area of great mutual interest and huge practical importance, this proposal aims to instigate research links that will lead to long-term collaboration between the two key research groups in a broad spectrum of overlapping research interests in complex fluid flows.

5. Modus operandi
We will operate in the following way. Each year we will hold a 3-day workshop: the first one will be in Princeton and the second one in Oxford. The visiting team will comprise 5 or 6 researchers, spanning faculty and junior members (postdoctoral researchers or Graduate Students), and will be chosen for compatibility with the topics under discussion. During the morning of each meeting, there will be presentations on current experimental work, and then the rest of the meeting will be devoted to brainstorming sessions on modelling. At least one junior member from the visiting team will then remain with the hosting team for several more weeks, in order to carry forward the ideas generated during the workshop. The first workshop will be dedicated to coagulation and flocculation and adsorption and ion exchange and Dr Ian Griffiths will be the member of the visiting team that remains behind. We anticipate that we will submit a joint grant application on the back of this visit, to employ Dr Griffiths once his current contract expires. The thrust of the second workshop will be decided during year 1.

We will also use the research ideas coming from these workshops as the basis for MSc projects (Oxford) and junior-year and/or Senior Thesis projects (Princeton).

References