**NGN PhD Studentship Proposal**

Note that proposals will be assessed against both the quality of the scientific content and of the proposed training experience.

**Proposed supervisors (lead first)** Prof. Michael Fairweather (Leeds)

*Industrial supervisor/partner* Dr. Steve Graham (National Nuclear Laboratory); Mr Geoff Randall (Sellafield Ltd); Manus O’Donnell/Laure Pellet (EdF); Robert Harrison (Rolls-Royce)

**Project Title** Particle Transport, Deposition and Agglomeration for Nuclear Reactor and Nuclear Waste Flow Applications

**Host Institution(s) and Department(s)/School(s)** University of Leeds, School of Process, Environmental and Materials Engineering

**Summary (250 words max; this will be used in recruitment publicity)**

Solid suspensions at various concentrations are encountered in many fluid flows of importance within the nuclear industry. They are of significance because of the requirement to be able to predict their mobility, flow rate and composition, and in assessing their potential to damage the systems through which they are conveyed. Mathematical models are of value in predicting the behaviour of such flows since the experimental investigation of all the flow characteristics and types of interest would be prohibitively expensive. Validated models can also be used to predict their transport behaviour to enable cost effective process design, to provide input to process selection, and to allow the prediction of operational boundaries, as well as in maximising the performance and safety of nuclear systems. Of particular interest in this project is predicting the behaviour of the solid particle-laden fluid flows of relevance to advanced nuclear reactor and nuclear waste processing operations. Large eddy simulation will be coupled with a Lagrangian particle tracking technique, with the methods to be developed capable of addressing all the inter-phase interactions of relevance, and more specifically the effect of the presence of particles on their deposition and re-suspension in such flows. Particles of different sizes and shapes, and suspensions of different concentrations, will be addressed. The models will be validated against available experimental data, with the proposed work increasing our understanding of, and ability to predict, these flows which is of value in improving the simpler modelling approaches conventionally used within industry.

**Introduction (250 words max)**

Nuclear power generation has an important role in the energy portfolio of the UK and worldwide, and solid suspensions at various concentrations are found in the many of the fluid flows encountered within the nuclear industry. Research and development are required to allow optimisation of the design and performance of nuclear systems, and improved safety, as well as the efficient disposal of waste. Of particular interest here is predicting the behaviour of nuclear reactors under steady state and accident conditions, as well as the flows encountered in nuclear waste processing operations. In particular, the formation, transport and deposition of particulates in a reactor coolant circuit are important considerations in maximizing the performance and safety of all reactor systems. In-circuit dust or "crud", arising from the spallation or oxidation of metal surfaces exposed to the coolant flow, is a potential source of accidental release of radiation to the environment, whilst its deposition and build up on reactor components has a significant impact on thermal efficiency and plant lifetime. Crud transport remains an outstanding issue, with the mechanisms initiating suspension of particles within a flow, deposition on surfaces, and eventually re-suspension requiring further investigation. Individual crud particles are small, but these generally agglomerate into larger particles giving rise to a wide range of sizes and morphologies. Similarly, nuclear waste sludges contain particles of a wide range of sizes and shapes, and their differing settling and re-suspension behaviour impacts on their mobilisation and transport characteristics, and hence the efficiency of processing options.

**Hypotheses, aims and objectives.**
Hypotheses
The number of variables and degrees of freedom of interest in the above applications is significant and this, together with the hazardous nature of the flows of interest, makes experimental studies prohibitively expensive and in many cases practically impossible. Experiments in idealised laboratory flows are possible, and indeed provide useful data for the validation of computer models and the elucidation of underlying physics, and such data will be used in this project where available. However, consideration of many practical flows must rely on predictions based on computational fluid dynamic techniques. Advances in computer technologies have led to significant developments in the area of computational fluid dynamics. This includes the development and routine use of direct numerical simulation (DNS), large eddy simulation (LES) and Reynolds-averaged Navier-Stokes (RANS) equation methods which, for particle containing flows, are coupled to Lagrangian particle tracking or Eulerian modelling approaches. At the present time the run times for DNS preclude its use in predicting the flows of interest, whilst RANS approaches, which solve averaged equations for the turbulent flow, cannot capture the detail and complexity of multi-phase flows required for their reliable prediction. At the present time LES, in which the large-scale turbulent motions are solved for directly, as a consequence gives more reliable predictions of flow turbulence, and hence offers the greatest potential for the accurate description of these flow. Additionally, although Eulerian approaches to modelling particle transport in turbulent flows are available, they lack the accuracy and precision of Lagrangian particle tracking techniques which can, as a consequence, be used to give a more detailed understanding of the flows in question.

Aims
- To establish a predictive model, based on large eddy simulation and a Lagrangian particle tracking technique, capable of predicting the deposition and re-suspension behaviour of non-spherical particles, including models for particle agglomeration, agglomerate break-up and particle-wall interaction.
- To investigate the behaviour of non-spherical particles of different sizes and shapes in ideal turbulent channel flows, contrasting their behaviour with that of spherical particles, with specific reference to particle deposition and re-suspension.
- To extend the applications work to more practically relevant flows in pipes and the annular space between concentric pipes.
- To validate the model predictions against available experimental data and, through collaboration with industrial partners, compare predictions of the model developed with industrial RANS approaches, with recommendations for improving the predictive accuracy of the latter.

Objectives
- Extend an existing Lagrangian particle tracking model to cover spherical particle agglomeration and break-up through implementation of hard sphere collision model and interaction forces applicable in gas and liquid flows.
- Extend particle tracking model to cover non-spherical particle shapes based on super-quadratic ellipsoid forms, formulating approach to handle resulting agglomeroid shape.
- Formulate particle-wall interaction model for non-spherical particles and agglomerates.
- Implement particle tracking model into large eddy simulation code, including stochastic Markov model to represent influence of unresolved fluid velocity fluctuations on particles.
- Idealised runs for channel flow exploring impact of particle shape and agglomeration on particle deposition and re-suspension behaviour. Explore impact of one-, two- and four-way coupling between fluid and particles.
- Runs for liquid flows in pipes (waste processing) and gas flows in annular space between concentric pipes (reactor flows), exploring deposition and re-suspension behaviour of non-spherical particles.
- Validate predictions against available experimental data in literature and to be gathered at University of Leeds and Xiamen University.
- Work with industrial partners to obtain RANS predictions based on spherical particle paradigm, and compare predictions with present model predictions. Propose means of improving simpler RANS modelling approaches.

Methodology and Approach (1000 words max)
The fluid flow in the channel, pipe and annulus of interest will be predicted using large eddy simulation (LES). The sub-grid scale (SGS) stress arising from the top-hat filtering operation on the Navier-Stokes equations will be modelled using the Germano dynamic approach, with a stochastic Markov model used to represent the influence of the unresolved fluid velocity fluctuations experienced by a particle. The resulting transport equations
will be solved using the computer program BOFFIN [1] to obtain the flow and turbulence characteristics. The code implements an implicit finite-volume incompressible flow solver using body-fitted and Cartesian coordinates and a co-located variable storage arrangement. Time advancement is performed using an implicit Gear method for all transport terms with variable time step, and the overall procedure is second-order accurate in space and time. For the convection terms an energy conserving discretisation scheme is used and matrix pre-conditioned conjugate gradient methods are employed to solve the equations for pressure and velocity. The code has been applied extensively in the LES of reacting and non-reacting turbulent flows, including multi-phase flows by the present author (e.g. [2, 3]).

The linear motion of stochastic particles in a turbulent flow field can be viewed as a random process with their position determined by two parts: a deterministic part obtained from known filtered LES velocities that contain the resolved scales of turbulence; and a stochastic component arising from the SGS turbulent motions of the fluid phase and Brownian motion. The deterministic part will be taken from the Maxey and Riley formulation for the force per unit mass, such as drag, lift forces and buoyancy-gravity forces. A stochastic Markov model will be used to represent the influence of the unresolved fluid velocity fluctuations. Particle rotation will be predicted using solutions of the Euler rotational equation accounting for the net torque exerted on a non-spherical particle caused by the non-coincident centres of mass and pressure, and the torque due to the resistance on a relatively rotating body. Transforming between the particle and inertial frames of reference makes use of the four Euler quaternions. Particle non-sphericity is then modelled through inclusion of the effects of linear motion in the inertial reference frame, and rotational motion in the particle frame, with differing particle shapes modelled using super-quadratic ellipsoid forms. The particle equations of linear and angular momentum will be integrated using a fourth-order Runge-Kutta method, coupled to a Lagrangian particle tracker. Further details may be found in [4].

The main developments in this project will be in relation to the agglomeration (and break-up) of spherical and non-spherical particles, and the particle-wall interaction model.

The relative motion between particles is affected by Brownian motion, fluid in-homogeneities such as shear and turbulence, and external forces such as gravitational, electrostatic and van der Waals forces. These factors determine the frequency of particle-particle collisions. The detection of the collisions will be deterministic and based on the hard-sphere model. Particle-particle interaction, also called the adhesion step, controls whether colliding particles will adhere or bounce off one another. The main adhesive forces are the van der Waals force, the electrostatic force and the force arising from the surface tension of adsorbed liquid films. The standard (i.e. without adhesion) hard-sphere model is based on writing equations for the impulse acting on the colliding particles formulated with the use of two additional parameters: the restitution coefficient, accounting for the loss of mechanical energy due to plastic deformation, and the Coulombian friction coefficient accounting for the particle surfaces sliding over each other during the collision. Two particles approach a collision with a specific velocity, with the normal and tangential components of the impulse used to model the interaction in the standard hard-sphere model. Additional impulse, acting due to adhesion interaction, is assumed to act normal to the plane of impact. The existence of the additional impulse means that the colliding particles enter a potential well, from which they may or may not escape depending on the mechanical energy lost during the collision due to dissipative processes, such as any plastic deformation of the particles during the impact. The agglomeration criteria are then obtained by comparing the momentum of the particles as they leave the collision with what is necessary to escape the potential well. A particle-particle agglomeration model will be built into the existing Lagrangian particle tracking routine based on the above approach by the student, with another consideration requiring further examination, specifically in relation to run time considerations, being the shape of the resulting agglomerate following particle collision.

A new particle-wall collision model will also be developed that aims to detect the point of collision by determining the closest particle surface to contact the wall. For a perfect sphere, this is well known. For ellipsoidal particles, the wall collision will be modelled based on the particle location and its orientation with respect to the wall. A particle is then said to have collided with the wall when the distance of the particle centroid from the boundary surface is within the range of the semi-minor axis and the semi-major axis, depending on its orientation relative to the wall. For arbitrary shaped particle, collision detection is complex but can be approximated by adopting the rough wall collision model.

Having developed the agglomeration and particle-wall interaction models as above these will be incorporated in the LES code and the overall model applied to studies of agglomerating particle deposition and re-suspension in the channel, pipe and annulus flows of interest.


### Programme of Work

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<th>Year 1</th>
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<td>Technical foundations and professional skills training</td>
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<td>Student-specific research training</td>
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<td>Familiarisation with existing large eddy simulation and Lagrangian particle tracking codes</td>
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<td>Validate predictions against available experimental data in literature and to be gathered at Universities of Leeds/Xiamen</td>
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<td>Comparisons between industrial RANS predictions and new approach, with recommendations for RANS model improvement</td>
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### Student Specific Training (500 words max)

The “Building Foundations” element of the student Study Programme will provide the student with a broad grounding across nuclear science and engineering, with professional development also provided through the Project Management- Professional Development Programme and the industry-led professional development short course. All this training will be provided through the Centre.

The remaining “Student-Specific Training” to be delivered at the University of Leeds will address academic, technical and professional training to develop specific skills. The University has recently reviewed strategy for researcher development and now has a new strategy and provider structure in place (see www.leeds.ac.uk/rtd). There is a researcher development team of three Faculty-based researcher development hubs and a Staff and Departmental Development Unit hub, alongside other central service providers including the Library, Information System Services and the Careers Service. These provide an extensive course programme covering a wide range of topics and skills such as: research methodologies and data management; techniques for information search and organisation; personal effectiveness and professionalism throughout the research process; strategy, project planning and management; ethics and intellectual property; good communications with a wide range of audiences for your research; and career management skills. This provision is guided by University strategy and national initiatives such as the Researcher Development Statement and Framework, the Researcher Concordat, and European HR Excellence in Research (awarded to the University in 2010).
In terms of this project, specific technical training will be required for the PhD student associated with the techniques to be developed and used. Additionally, nuclear-specific training would also be beneficial in terms of the applications work. The University has existing modules at Levels 3/4 MEng/MSc level that could appropriately used for training purposes. Relevant technical modules include: PEME3611 Particle Process Engineering; PEME5310M Multi-Scale Modelling; PEME5350M Computational Transfer Processes; CCFD5100M Finite Differences and Control Volume; CCFD5110M Incompressible Flow; CCFD5130M Reaction Fronts and FORTRAN; CCFD5140M Finite Elements and Boundary Elements; CCFD5170M Commercial Software; CCFD5200M Advanced Commercial Software; and CCFD5300M Turbulence and Two Phase Flow. Additionally, new modules on mathematical modelling, numerical solution methods and computational fluid dynamic software training, including the use of high performance computing, are also being developed now for roll out in September 2014. More general nuclear applications modules include: PEME3361 Nuclear Fundamentals; PEME3371 Nuclear Operations; PEME5395M Nuclear Futures; and PEME5384M Nuclear Engineering and the Nuclear Industry.

Courses and modules from the above would be selected to give broad, project-relevant nuclear training, professional and specific technical training in numerical modelling and multi-phase flows, dependent on the background of the student. Additionally, links with Xiamen University, of value to the technical progress of the project as noted below, would be extended through attendance by the student at their 2 week Summer School on Clean Energy Science and Engineering (which contains a significant nuclear component), held jointly in China with the University of Leeds and the University of Michigan, which includes tours of nuclear power plant and decommissioning faculties.

**Track record (500 words max)**

Prof. Michael Fairweather graduated from the University of Leeds with BSc and PhD degrees, and subsequently joined British Gas where he worked on a range of projects of relevance to the efficiency, safety and environmental impact of gas use. He rejoined the University of Leeds in 1998, being promoted to a Chair in Thermofluids and Combustion in 2005. His research interests are in the areas of fluid dynamics and combustion, with particular emphasis on the development and use of computational fluid dynamic techniques, and experimental measurement. Prof. Fairweather has authored more than 220 peer reviewed publications, was the recipient in 2010 of the IChemE Frank Lees Medal awarded by their Safety and Loss Prevention Subject Group, and has been associated with research grants supported by the EPSRC, EC, industry and government sources worth £8.2M since joining the University. He was involved in the EPSRC’s Keeping the Nuclear Option Open (KNOO) and Decommissioning, Immobilisation and Management of Nuclear Wastes for Disposal (DIAMOND) projects, and is a member of their new Decommissioning, Immobilisation and Storage Solutions for Nuclear Waste Inventories (DISTINCTIVE) project. He also holds grants from the EPSRC on the Computational Modelling for Advanced Nuclear Power Plants, and Thermal Hydraulics for Boiling and Passive Systems, as well as being a member of the Advanced Fuels for Generation IV Reactors, EC FP7 project and Leeds PI of the TSB project on the Measurement and Modelling of Sludge Transport and Separation Processes. Together with staff of Xiamen University, he is also a member of the China Prosperity Strategic Programme Fund, Technological Assessment of Building Nuclear Waste Disposal Reservoirs project funded by the Foreign and Commonwealth Office. He has undertaken a number of research projects funded entirely by the nuclear industry, and routinely carries out consultancy work on their behalf. He is a member of the management committees of the National Nuclear Laboratory-University Centre for Collaborative Research, the Sellafield Ltd-University Sludge Centre of Expertise, and the University Centre of Excellence in Nuclear Engineering. Of relevance to all these activities he has expertise in modelling and simulation (RANS, LES and DNS of single- and multi-phase flows) and experimental studies, with application to the nuclear fuel cycle, waste management and decommissioning, and reactor flows, and to severe accident and nuclear safety issues (dispersion and build-up of flammable and particulate releases, their subsequent ignition and the consequences of any resultant fire or explosion).

LES and Lagrangian particle tracking techniques to be used in the work proposed are being developed and used on a number of the projects noted above. Non-spherical particle dynamics are also being considered, although application of all these techniques to agglomerating spherical/non-spherical particles and their deposition and re-suspension behaviour, the focus of the present work, is not. The various projects noted above will also provide the PhD student with significant networking opportunities in areas of relevance to applications of the work proposed.
### Relevance to beneficiaries (250 words max)

The work proposed will deliver fundamental understanding of particle-laden flows of interest to nuclear reactor operations, nuclear waste clean-up and decommissioning, and as well as to those involved in general waste disposal and water treatment. Additionally, fluid flows containing solid particles are encountered in, and are of fundamental importance to, manufacturing in the chemical, pharmaceutical, healthcare, biomedical, fuel, personal product, mineral and new materials sectors. In all these applications, an understanding of how particles interact with and within fluid flows is necessary to allow the optimisation and performance improvement of existing equipment and processes, the identification and solution of operating problems, the evaluation of retrofit options, and the design of new equipment, systems and plant. Also, most natural dust, solid aerosol and waste particles generated in industrial processes are non-spherical. In providing a basic understanding of the flow behaviour, settling and re-suspension characteristics of such particles, the project is of broad relevance to others working in the UK academic sector on multi-phase flow problems in all the above application areas, and to those developing techniques for their prediction. The understanding and predictive methods to be developed are also of interest to the nuclear industry in establishing the characteristics of particle-laden flows for use in the design of safe and efficient reactors, and effective waste management processes, and to assist in the identification of opportunities to accelerate the UK’s decommissioning programme. They are also more generally relevant to all those industrial sectors noted above that use fluid flows containing solid particles.

### Impact (250 words max)

Results will be made generally available through conference and journal publication. The work described is at a generic level, although with specific nuclear-related applications. As an investigator on EPSRC projects in both reactor and waste flow areas, the applicant has regular meetings with both academic and industrial colleagues who will benefit from the work. In particular, the DISTINCTIVE project plans to hold regular meetings with industrial and governmental stakeholders, with the same already the case with the EPSRC Nuclear Power Plant and TSB Sludge Transport projects noted above. These projects also use other means to engage stakeholders, disseminate information and encourage knowledge transfer, including newsletters, web-sites, reports and training programmes. More specifically, industrial project partners would benefit from regular project management meetings used to influence the direction of the work, and from comparisons between their modelling techniques and the more advanced methods to be developed, with the project outputs of direct benefit in improving the accuracy and applicability of the former approaches. The applicant has further links to the nuclear industry through his management committee memberships of the NNL and Sellafield Ltd centres noted. All these close and ongoing relationship with the industry have led to knowledge transfer through the delivery of experimental data, theoretical modelling techniques, and design tools and recommendations. Importantly, knowledge transfer is also taking place through the recruitment of PhDs into the industry, and via direct consultancy activities which I have been involved in with various nuclear companies for over 5 years.

### Networking (250 words max)

The student would interact on a regular basis with industrial project partners through management meetings used to influence the direction of the work, and to discuss related technical issues, and would benefit from their advice and technical expertise. Comparisons between industrial modelling techniques and those to be developed would also hopefully extend networking opportunities into the companies involved. The student would be invited to technical project meetings associated with the EPSRC DISTINCTIVE and Nuclear Power Plant projects, and the TSB Sludge Transport project, noted above given the relevance of both experimental and numerical modelling work being undertaken on those projects to the proposed work. This would be useful in improving networking with both academic and industrial colleagues, and of particular relevance would be links to the groups of Prof. Mike Reeks (at Newcastle University) and Prof. Dominique Laurence (at the University of Manchester) who are undertaking complementary work on nuclear reactor flows. Experimental work of relevance to model validation is also ongoing at the University of Leeds, but data should also be available through our collaboration with Xiamen University in China (Dr. Jun Yao) who are also undertaking related numerical simulation work. This would involve trips to China to assist in their experimental programmes and the collection of data, and interaction on numerical simulation activities. The opportunity to interact with other NGN PhD Studentship projects would also be welcomed.