

8th Annual PGR Conference

BEAR

ABSTRACT BOOK

23rd February, 2018

8th BEAR PGR Conference Timetable

Time	Event	Speaker
09:30	Opening Address	Prof Jean-Baptiste Cazier
09:35	Keynote	Karl Podesta / Microsoft
10:05	PGR Presentation	Joshua Allen Use of First-Principles Calculations to Determine Planar Fault Energies in Superalloys
10:25	PGR Presentation	Valter Jantara Junior Wind turbine gearbox damage simulation
10:45	Coffee Break	
11:00	PGR Presentation	Syeda Anam Hashmi Aerodynamics of a passenger train against different types of windbreak walls under crosswinds
11:20	PGR Presentation	Rana Moeini Failure Detection of Power Electronic Module Through Measurement of Thermal Sensitive Electrical Parameter
11:40	BEAR User Forum	
12:25	Q & A + Lunch	
13:25	Keynote	Rob Hoehndorf / King Abdullah University of Science and Technology
13:55	PGR Presentation	Shen Huo Numerical Analysis on the Flow Structure of a Tornado-like Vortex using Large Eddy Simulation
14:15	PGR Presentation	James Shaw Probing Structural Hierarchy in Colloidal Gels
14:35	Coffee Break	
14:50	Keynote	Andrew Edmondson Research Software Group Leader IT Services, University of Birmingham
15:20	PGR Presentation	Lazaros Melidis Supramolecular Recognition of Nucleic Acid Structures Found in Viruses
15:40	Coffee Break	
15:55	PGR Presentation	John Hey Isomers and Energy Landscapes of Micro-Hydrated Sulfite and Chlorate Clusters
16:15	PGR Presentation	Grigorios Papatzikas Using Birmingham Environment for Academic Research (BEAR) to understand the metabolic regulation in haematological cancers
16:35	Ending Ceremony	Prize presentation for posters and talks



Aerodynamics of a passenger train against different types of windbreak walls under crosswinds

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Effects of external aerodynamics on high-speed trains are usually pronounced under strong crosswinds [1]. This research aims to explore both experimentally and numerically the influence of windbreak walls as a preventive measure on the flow around trains subjected to crosswinds in order to propose the best possible design for an effective windbreak wall. The experimental campaign comprises of measuring surface pressures on a 1:25 model-scale of Class 390 Pendolino train under varying yaw angles with different windbreak walls. Numerical simulations will be performed to understand how the flow around the train is affected by the different type of windbreak walls. Experimental results will be used to provide validation to numerical simulations. Numerical simulations would involve the use of different turbulence models, applying different boundary conditions and using different simulation models. The sensitiveness of different discretization methods, turbulence models and computational grids will be discussed. Flows with high Reynolds numbers around trains under crosswinds are expected mainly due to; stagnation and impingement, formation of boundary layers on curved surfaces of the vehicle and due to vortex shedding from the roof and underbody of the vehicle. It can be anticipated that the results for the overall mean aerodynamic side and lift forces along with rolling moment coefficients will be sufficiently accurate for the stationary experiments. Additionally, it can be established already that the height of the windbreak wall, distance between the windbreak wall and railway tracks and the design of the windbreak wall can significantly influence the flow around a train.

References

[1] Diedrichs, B. (2003). **On computational fluid dynamics modelling of crosswind effects for high-speed rolling stock**. Proceedings of the Institution of Mechanical Engineers, Part F: Journal of Rail and Rapid Transit 217: 203.

Keywords: Computational Fluid Dynamics (CFD), Numerical simulations, Train aerodynamics

FAILURE DETECTION OF POWER ELECTRONIC MODULE THROUGH MEASUREMENT OF THERMAL SENSITIVE ELECTRICAL PARAMETER

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Background

Anticipation of failure mechanisms in different parts of wind turbines can offer a condition monitoring systems. Power electronic converters encounter severe thermal stresses due to wind speed variations. Insulated gate bipolar transistors (IGBT) modules are the most vulnerable parts of the power electronic converters [1]. Temperature profile can be a failure detector of IGBT modules. However, direct measurement of temperature is not possible without changing the IGBT module instruction.

Methods

Switching parameters of IGBTs can be an alternative to be a proper failure detector. However, the accuracy of TSEPs-based method in order to detect failure mechanisms of IGBTs within the operation of converter is not clear. The built converter is used to study the sensitivity of switching parameters to the variation of load and temperature, Figure.1. Switching parameters are measured in healthy mode of IGBT within the operation of the built converter. Switching time parameters of IGBT is determined based on time difference between gate emitter voltage (V_{GE}) and collector current, Figure.2.

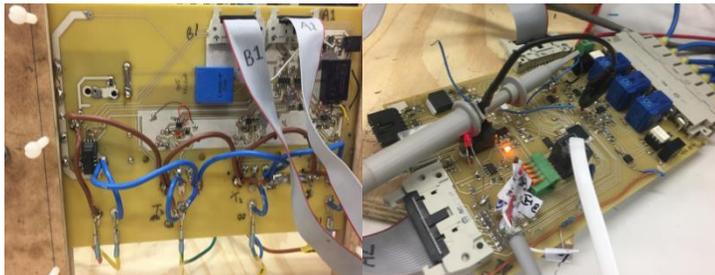


Figure.1. Power and controller board of the built three-phase converter

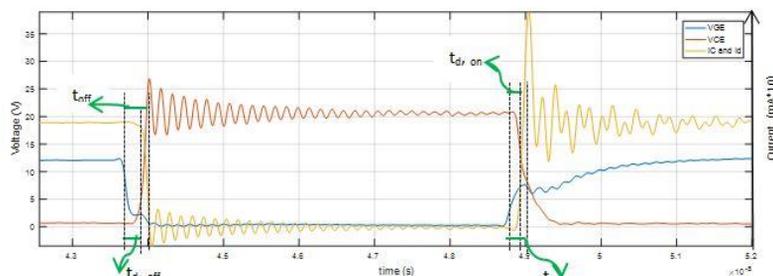


Figure.2. Switching time definition

Supramolecular recognition of nucleic acid structures found in viruses

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Background

We have developed a new class of nanosized supramolecular agents (cylinders) that recognise in a novel shape specific way some RNA and non canonical DNA structures notably Y-shaped junctions and bulge structures. Preliminary work has demonstrated that this gives rise to novel antiviral and antibiotic action. For example, our agents recognise a specific bulge structure in the trans activation response region of HIV-1 RNA and inhibit HIV replication in mammalian cells without otherwise damaging the cells.

Methods-Results

The binuclear cylinders have centres of Ru, Fe, Ni or Co, which raises a challenge for computational studies, since the classical molecular dynamics (MD) cannot take into account the electronic structure of the molecule. Given the presence of embedded transitional metals in the cylinder, Density Function Theory and Molecular dynamics/DFT hybrid needs to be employed for geometry optimisation and non-covalent interactions in extended nucleic acid-cylinders systems. Once the optimisation and in silica characterisation of the series of cylinder variants is done, one can start simulating the interaction with RNA and DNA structures with linear scaling DFT or QM/MD. We are using NWChem and CP2K for the DFT optimisation and calculations of the electrostatic surface potential. Both packages support QM/MD runs that will be used later in higher scales.

Keywords:

Bioinorganic chemistry, DFT, DNA/RNA

Study the Mixing of non-Newtonian Fluids Using Positron Emission Particle Tracking

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Background and Methods

Previous studies on mixing of floating particles in mechanically agitated vessels focused mainly on power saving by achieving lower just-drawdown impeller speeds and on the performance of different impeller and baffle configurations. The internal flow field and spatial dispersion of floating particles have been little studied experimentally. Owing to the opaque nature of such suspensions, work has been restricted to flow visualisation through the wall and measurement of cloud depth. In this work, the technique of **Positron Emission Particle Tracking (PEPT)** was used to investigate at the just-drawdown speed the two-phase flow field inside a stirred vessel of polypropylene particles of 3 mm diameter and 900 kgm^{-3} density in fluids of Newtonian, shear-thinning (SN) and shear-thickening (ST) rheology. Mechanical agitation was achieved by a six-blade down-pumping pitched blade turbine (PBTD).

Results and Conclusions

For the first time, the effects of the fluid rheology on the two-phase flow pattern and 3D phase velocity and concentration fields were determined for different impeller submergence levels ($S = T/4, T/3, T/2$ and $2T/3$) in a fully baffled vessel. Comparisons between impeller submergence levels in all fluids revealed that lowering the impeller to $S \geq T/2$ invariably produced a more homogenous suspension. The liquid and solid phase velocity distributions allowed estimations of the spatial distribution of particle-fluid slip velocities in the vessel. These data were used to assess, for the first time, the magnitude of the likely error involved in local mass transfer predictions using Frössling-type correlations which are based on the particle settling/rising velocity.

Keywords: Mixing, Rheology, Floating Particles

Isomers and Energy Landscapes of Micro-Hydrated Sulfite and Chlorate Clusters

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Abstract

Ions can be classified according to the Hofmeister series, ions which induce disorder within the hydrogen bonding network of water and disrupt protein stability are labelled as chaotropes, whilst ions which promote order and protein stability are classified as kosmotropes.¹⁻⁶ The hydration of ions is important as it has bearing on the atmospheric nucleation of water clusters and other areas of atmospheric science.⁷⁻⁹ We have previously studied the chaotropic perchlorate (ClO_4^-) and the kosmotropic sulfate (SO_4^{2-}) ions in finite gas phase water clusters.¹⁰⁻¹²

SO_2 released to the atmosphere is quickly oxidised to form sulfur(IV) and sulfur(VI) species. Sulfite (SO_3^{2-}) and other sulfur(IV) ions are commonly found in inorganic aerosols, which are important in atmospheric science as they contribute to the formation of acid rain.^{8,13-15} Chlorate (ClO_3^-) is isoelectronic with sulfite and shares a similar geometry, with a lower charge and thus provides a useful comparison.

We present putative global minima for the micro-hydrated sulfite $\text{SO}_3^{2-}(\text{H}_2\text{O})_N$ and chlorate $\text{ClO}_3^-(\text{H}_2\text{O})_N$ systems in the range $3 \leq N \leq 15$ found using basin-hopping with an empirical potential. We present a structural analysis of the hydration of a large number of minimised structures for both hydrated ions in the range $3 \leq N \leq 50$.

We show that sulfite is a significantly stronger net acceptor of hydrogen bonding within water clusters than chlorate, strongly suppressing the appearance 'dangling' OH bonds in low energy clusters.

We also present an qualitative analysis of a highly explored energy landscape in the region of the global minimum of the 8 water hydrated sulfite and chlorate systems.

References

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Comparative study of lattice and tubular steel wind turbine towers

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Background

Wind energy has been one of the most developing forms of sustainable energy production. The commonest wind power converter is the one based on the cylindrical steel tower. Research on the structural optimization of wind turbine towers is of great interest and importance and aiming to contribute to better understanding of the structural behaviour of alternative types of wind turbine towers, the research work focuses on the development of reliable numerical models in order to predict accurately and interpret the structural response of both shell and lattice towers.

Methods

The wind turbine tower that is used for the comparative study of wind turbine tower design has a total hub height of 76.15 meters. The tubular tower consists of 3 parts that are modelled with reduced integration shell elements S4R as described in the software manual [3]. The lattice tower used for the comparative study shares the same height as the tubular one. The structural sub-systems that the tower consists of have distinct roles in the load transfer mechanism of the tower. Each sub-system is investigated and optimized separately and the angle of the diagonals of the V shaped bracing are investigated towards minimizing the total weight of the structure.

Results

Regarding the tubular tower, material nonlinear analysis is performed to examine the tower response towards this combined loading. The tower shell thickness is optimized and a calculation of the total material used is also performed. As far as the lattice tower is concerned, all the tower subparts are designed and the optimum tower configuration is selected in order to minimize the total material used along with maintaining the tower load bearing capacity. The lattice tower is lighter compared to the tubular tower for the selected hub height and critical assumptions can be made towards wind turbine tower optimal design.

Conclusions

The present study investigates the potential of substituting tubular wind turbine tower with lattice ones with the project of minimizing the total structure weight while maintaining the structure load bearing capacity.

References

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Keywords:

Wind turbine towers, steel structures, numerical analysis

Wind turbine gearbox damage simulation

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Background

Global wind power capacity has been annually growing at a rate of around 20% over the past years and has thus become the most important renewable energy source in the world [1]. However, reliability issues still restrict the expansion of wind turbine industry. Among several operational challenges, wind turbine gearbox reliability appears to be most important one since most gearboxes only survive 30% of their predicted design lifetime of 20-25 years [2].

Methods

Different materials used in the manufacturing process of wind turbine gearboxes have been evaluated. The damage mechanisms affecting gears have been investigated based on metallographic analysis of failed samples removed from in-service industrial wind turbines. Finite element analysis has been carried out to simulate damage initiation in wind turbine gearboxes and compare it with the damage seen in the samples retrieved from the field.

Results

Wind turbine gearboxes can suffer from several conditions such as instant misalignments which eventually lead to lubrication starvation and failure. Different types of misalignment were simulated via finite element analysis.

Conclusions

Angular misalignment appears to be the most detrimental cause of damage in wind turbines gearboxes, however, factors such as lack of lubrication may also play a role.

References

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Keywords:

Wind energy, finite element analysis, gearbox

Numerical Analysis on the Flow Structure of a Tornado-like Vortex using Large Eddy Simulation

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Tornadoes are some of the most horrifying natural disasters known to men and can cause tremendous damages to civil structures. The structure of a tornado-like vortex is numerically simulated using the LES turbulence model. An analysis on the flow reveals the tornado-like vortex to be at a turbulent state where the swirl is much weaker at the centre but reaches a peak at the boundaries of the vortex. At the centre of the vortex is a turbulent core with chaotic downdraft flow that penetrates the entire vortex but breaks away before touching the ground, forming a recirculation zone. A critical region at the boundary layer of the ground is where all the maximum velocity components occur. Some oscillations can be observed and were analysed with power spectrum analysis to quantify the swirl motion of the flow structure, revealing a periodic motion in the clockwise direction with the magnitude of 0.035 meters with the period of 1.375 seconds. The mean flow field appears to be axis symmetrical, indicating the dynamic structure of the vortex to be stable. Flow fields are matched with full scale data of naturally occurring tornadoes to reveal the velocity and length scales of the tornado-like vortex.

References

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Keywords: tornado-like vortex, large-eddy simulation, vortex core, power spectrum analysis

Use of First-Principles Calculations to Determine Planar Fault Energies in Superalloys.

Talk Abstract By Joshua Allen

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Since their discovery superalloys have become a mainstay of the aviation industry due to their use in turbine blade applications and have also found a series of uses in other industries such as fossil fuels. It is of key importance to create superalloys which can sustain higher temperatures for longer periods of time due to the large increases in fuel economy and efficiency that even a small increase in temperature (of a turbine in operation) could yield. Superalloys derive their strength from a two phase γ/γ' microstructure.

Superalloys are most commonly based off Nickel but in recent years Cobalt based alloys are making a resurgence due to the discovery of alloy compositions which also exhibit the highly desired γ/γ' microstructure by Sato et.al in 2006[1].

Superalloys have a variety of exceptional properties such as hot corrosion and impact resistance, but obtain their prefix super from the occurrence of the yield stress anomaly (YSA). Of key importance to the YSA are the energies of the planar fault type known as the Anti-Phase Boundaries (APBs). This in addition to the superlattice intrinsic stacking fault (SISF) are highly relevant to enhancing the creep properties essential to service life.

The main thrust of this research is to determine how these fault energies are impacted on by compositional changes using highly accurate first-principles calculations in the Vienna Ab-initio Simulation Package (VASP) program to design more advanced superalloys. Such calculations require high amounts of computational resources which is where the BEAR supercomputer has proved invaluable.

Keywords: Superalloys, Planar Faults, Vienna Ab-initio Simulation Package, Creep, Yield Stress Anomaly, First-Principles.

References: [1] Cobalt-base high-temperature alloys. 2006. J Sato, T Omori, K Oikawa, I Ohnuma, R Kainuma, K Ishida. Science. 312(5770). 90-91.

Probing Structural Hierarchy in Colloidal Gels

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Background

Gels are disordered soft materials of much industrial relevance [1]; governed by competing interparticle interactions where an interplay between short-ranged attraction and relatively long-ranged repulsion is crucial, the morphology of these systems is highly sensitive. Colloidal suspensions provide useful model systems to further our understanding of cluster formation, gelation, and crystallisation because of the scope for tuning interparticle interactions. This project seeks to investigate dynamical pathways for cluster and gel formation of both isotropic and anisotropic colloidal particles functionalised in a variety of synthetically-accessible ways [2].

Methods

A coarse-grained description for the colloidal particles is used with effective potentials, where the solvent degrees of freedom are treated implicitly. The project currently employs Brownian Dynamics and uses the tools of statistical mechanics to investigate the dynamics of colloidal matter in this context. We also investigate the pathways to formation and the structures formed using a variety of computational techniques developed both in-house and externally.

References

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Keywords:

Colloids, Soft Matter, Simulation, Gel, Crystallisation

GWAS for tumour size, grade, stage, and age in NMIBC patients in West Midlands Bladder Cancer Prognosis Programme

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Background

Non-muscle-invasive bladder cancer (NMIBC) exhibits high recurrence and progression rates, causing significant burden on patients and healthcare systems. Current prognostic tools make use of tumour characteristics at the time of diagnosis, but fail to make an accurate prognosis on an individual level. We have performed a genome-wide association study (GWAS) to investigate associations with tumour size, stage, grade, and age at the time of diagnosis that could potentially improve the precision of prognostic tools used in clinical practice.

Methods

653 patients from the West Midlands Bladder Cancer Prognosis Programme (BCPP) had their biological samples genotyped and passed quality control procedures. Eagle v2.3.2 was used to estimate haplotypes, followed by imputation with IMPUTE2, using 1000 Genomes Phase 3 data as a reference panel. Single-nucleotide polymorphisms (SNPs) were tested using SNPTEST v2.5.2 for associations with all endpoints (tumour size (continuous (cm) and categorical (sample mean as a cut-off) outcome), stage (Tis and T1 vs Ta), grade (G3 vs G2 and G1), age (continuous (years) and categorical (sample mean as a cut-off)), filtering for minor allele frequency (MAF>0.01%) and imputation accuracy (info>0.3). Promising findings were tested in a sample of the Netherlands Bladder Cancer Study (NBCS).

Results

61 novel associations across all outcomes have yielded genome-wide significance ($p < 5 \times 10^{-8}$), corresponding to 29 distinct loci. In a meta-analysis of both cohorts, one SNP showed a promising association with tumour size, (rs180940944 ($\beta = 0.9$ cm, $p = 2.92 \times 10^{-9}$)), which is situated in an intronic region of the *NBEA* gene.

Conclusions

Our study adds novel findings to the current knowledge regarding associations between genetic variation and NMIBC characteristics at the time of diagnosis. Such findings may be useful for improving prognostication.

Keywords: Genome-wide association study, non-muscle-invasive bladder cancer, prognosis, recurrence

Metabolic characterization of Burkitt (BL) and Diffused Large B-Cell Lymphoma (DLBCL) cell lines as studied by cell extraction ¹H-NMR spectroscopy.

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Background

Alterations in metabolic processes that drive cells in aggressive malignant progression is now considered a new hallmark of cancer. Here, we investigate if changes in metabolic pathways can enlighten the grey area in mature aggressive B-cell Non-Hodgkin lymphomas (NHL) that arise from germinal centres of lymph nodes.

Methods

Untargeted ¹H NMR data has been acquired from three BL and three DLBCL cell lines to identify their metabolic profiles. Multivariate and univariate analysis was performed to distinguish BL from DLBCL and to identify up regulated metabolites for pathway analysis.

Results and conclusions

Partial least squares – discriminant analysis (PLS-DA) model can distinct BL from DLBCL cell lines. In pathway analysis the alanine, aspartate and glutamate pathway was significantly enriched in BL, which indicates that catabolism of these amino acids, may support the high proliferation rate of BL cells. On the other hand DLBCL cell lines seems to be more dependent on glycolysis and pyruvate metabolism to fuel their energy demands. Finally, up-regulation of taurine in DLBCL cells lines indicates a potential role of this metabolite as a biomarker to separate BL from DLBCL cases.

References

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Keywords:

Metabolism, NHL, BL, DLBCL, NMR.

