Imperial College London

UNIHEAT

2016 President's Medal for

Outstanding Research Team

Awards for Outstanding Research Team celebrate the achievements of research teams at Imperial, recognising outstanding research that delivers impact, a team's international standing and their beneficial contribution to Imperial.

Professor Alice Gast, President

The President's Award for Outstanding Research Team	The Award for Outstanding Research Team aims to celebrate the achievements of research teams at Imperial. Winning teams are selected based on the strength of evidence for: Outstanding research that delivers impact within and across disciplines International standing in research field/theme Impact and beneficial effects to Imperial College London Multidisciplinary teams are particularly encouraged to be considered for an award.	Eligible teams are those of at least five staff members, led by an Imperial academic at lecturer grade or above.

UNIHEAT Project Team

Team

The Imperial team includes:

Prof. G. F. Hewitt	Two phase flow; Heat Transfer; Crude oil fouling measurement.
Prof. G. Jackson	Thermodynamics modelling of the phase behaviour of crudes and their blends
Prof. S. G. Kazarian	Oil and deposit chemical characterization via advanced imaging
Prof. S. Macchietto	Heat Exchange & pipelines modelling and design; whole system integration
Dr. C.N. Markides	High-efficiency heat recovery, re-use and/or conversion to power
Prof. O. K. Matar	Fluid Dynamics and Rheology
Dr. M. Millan-Agorio	Oil and deposit physical characterization; catalytic upgrading
Prof. E. Muller	Thermodynamics modelling using molecular simulation
Dr. F Coletti	Industry Engagement Manager; crude oil fouling simulation

Each member has consolidated experience in his sector and is well recognised internationally.

The team is led by Prof Macchietto, the Project's Imperial Director and Chairman of the Steering Committee. His research focuses on the development and application of mathematical methods to process design, control and operation; model-based experiment design techniques for rapid model development and validation; and the use of systems methods for the development and optimisation of sustainable energy systems. He has co-authored >200 papers and is a frequent keynote speaker. At Imperial College he co-founded and was a director of the interdisciplinary Centre for Process Systems Engineering, of the Energy Futures Lab and launched a highly innovative MSc is Sustainable Energy Futures.
Advisory positions include membership of the Evaluation Committee of the Politecnico di Torino, Italy (part of its supervisory body), Advisory Board of ENSIACET (Institut National Politechnique), Toulouse, France, and Scientific Committee, Institut Mines Telecom, Paris (a grouping of all Ecoles de Mines in France). Appointed by the German Minister for Science to the Evaluation Committee for the German Programme for Excellence (2012).

He co-founded and lead 2 spinouts (Process Systems Enterprise Ltd – engineering software and services, which he led (twice) to the Sunday Times-TechTrack 100 list of Britain's fastest-growing unquoted companies; and Hexxcell Ltd – heat transfer software and services). Sandro was made Cavaliere of the Order of Merit by the Italian President, Italy's highest civil honour, in 2003. Awards include the McRobert Award 2007, top prize for

innovation of RAEng.; Rector's Award for Excellence in Leadership and Management - Imperial College (2008); IChemE Industry Awards for Innovation and Excellence -Education and Training (2009); Queen's Award for Enterprise–Innovation (with PSE); and Queen's Award for Excellence (with CPSE). He is a Director of the Asia Pacific Technology Network (international seminars).

Other members of the Steering Committee include Prof O.K. Matar and Dr. Paul Docx (presently Simon Hepworth) for Imperial College and for BP Dan Coy (Program Manager, BP Refining & Logistics Technology).

Prof. O K Matar's (OKM) group conducts world-leading, fundamental research in transport phenomena and interfacial flows with a wide range of applications that spans many length- and time-scales. Co-authored >150 journal articles, with over 2500 citations (h-index 29), including highly-cited papers on the breakup of surfactant-laden threads, thin electrified films, evaporating films and drops containing nanoparticles with moving contact lines, and nonlinear dynamics of two-fluid flows. 42 invited lectures, Editor-in-Chief of Multiphase Science & Techn., Assoc. Exec. Editor of J. of Engin. Mathematics, on Editorial Board of Intern. J. of Multiphase Flow, J. of Engrng, and Heliyon. Funding (over £20M) by EPSRC and industry includes the largest UK grant in fluid dynamics (http://www.memphis-multiphase.org/).

Nomination Overview

About 6% of the energy content of each crude barrel processed in a refinery is used in the refinery itself, globally equivalent to Exxon + ½ of Shell just to operate the world's 720 refineries, and producing 2.5% of manmade CO2 (just below aviation).

The UNIHEAT project, led by Prof Macchietto, brought together 5 distinguished researchers from the Boreskov Institute of Catalysis (BIC) in Novosibirsk with 8 academics from in Chemical Engineering, Imperial College London (ICL) and their teams (up to 60 researchers and 3 technicians) to execute an ambitious programme of research and technology transfer. UNIHEAT researches and develops innovative solutions and technologies to increase efficiency in the use and recovery of thermal energy and catalytic processes in the oil and gas, particularly refining, and chemicals industries, with particular focus on understanding of oil and oil deposition on thermal surfaces (fouling).

To overcome a plateau in research, one of the largest (and arguably the best) multidisciplinary teams in this area worldwide was assembled, integrating deep expertise in a number of adjoining fields (from molecular modelling to thermodynamics, fluid dynamics, reaction engineering and heat transfer, to the most advanced modelling, simulation and systems optimization methods) into a coherent approach and a joined-up research programme organised in 6 Themes to address and solve the fouling and energy recovery problems using a "whole system" approach. The Themes are

1 – Multi-scale modelling of crude oil fouling: from molecular to plant scale
2 – Characterisation of physico-chemical properties of oil and deposits
3 – Heavy Oil Catalytic Upgrading
4 – Thermodynamic power generation cycles for improved efficiency
5 – Drag reduction in pipelines
6 – Laser induced pyrolysis of light hydrocarbons

Theoretical research and multi-scale modelling are supported by an array of state-of-the-art equipment for measurement of unprecedented precision, observing ill-understood phenomena from new experimental windows across all scales, from in-situ nanoscale to industrial scale equipment.

In parallel, a dedicated Industry Engagement Programme (IEP) team of 4, supplied and managed by Imperial Consultants address project management, developing contacts with industry, feasibility studies, dissemination

and business development, so as to ensure “by design” relevance, applicability, transferability and impact of the research.

Supervision and coordination is provided by a Steering Committee, representing the key project stakeholders.

This is a rather complex project, with many challenges: opening up a new frontier for the college with Russian partners; the integration of disparate disciplinary skills towards solving a long standing, scientifically challenging problem (oil characterisation and refining efficiency). It also proposed (and delivered beyond reasonable expectations) an integrated, seamless approach between research, development, applications and technology transfer, involving (just on the college side), research (Chem Eng department and Research Contracts), Imperial Consultants, Imperial Innovations, and, in the last few months, the college’s Enterprise office.

Outstanding Research

This 3-year project, started on 2nd July 2012, was Imperial’s first sizeable project with a Russian partner. The team secured a US$14.6m grant (60% for Imperial) with funding from the Skolkovo Foundation (an agency promoting innovation in Russia) and BP, who joined in December 2012.
https://www.youtube.com/watch?v=gYzx1Q2Mv4Y http://www.bloomberg.com/news/articles/2011-12-21/bp-to-set-up-energy-efficiency-research-with-russia-s-skolkovo

A legal “consortium” agreement framework was achieved that enables all parties to work in an open way and new industrial partners to join in, covering up- front all intellectual property and revenue sharing issues to the satisfaction all partners. Given the complexities involved, this was itself a remarkable achievement.

The Imperial, BIC and BP teams meet in regular workshops alternating between Russia and UK, with frequent researcher exchanges in between, generating common understanding and fruitful collaboration.

In the first two years (of which 6 months for start-up), research output includes the publication of 31 journal papers, 49 presentations at conferences and 16 MSc dissertations. A significant number of innovative results were produced in each of the research Themes. A few highlights (of mainly the Imperial Team) include:

- significant progress in modelling crude oils and phase diagrams for mixtures using thermodynamic and molecular modelling, combined with data from SAXS scattering experiments. Coarse-grained models for toluene and heptane are being tested and validated against predictions obtained from Molecular Dynamics simulations
- novel results on the characterisation of crude oils and deposits using a unique range of advanced spectroscopic and chemical imaging methods (ATR-FTIR, NMR, ESR and SAXS), including the first in-situ measurements of several oils (supplied by BP), leading to new insights on the behaviour of oil at different spatial and temporal scales, deposit formation and oil blends stability.
- a novel batch reactor has been designed for rapid tests for fouling behaviour of crude oils and crude blends. Target molecules and syntheses for synthetic “asphaltene model compounds” were defined.
- a new Computational Fluid Dynamic model and a series of 3D CFD simulations highlighted the impact of wall surface temperature, bulk flow velocity and ageing on fouling formation rate and removal rate.
- modelling work at the equipment-scale produced a first approach to deposition on the shell-side of shell-and-tube exchangers, extensions to account for inorganics in the fouling deposits and cleaning operations and an initial attack of the desalting process.
- a project on drag reduction for pipelines has produced a complete new concept demonstration, two Case Studies for existing pipelines, working prototypes of catalytic heaters including improved catalyst

and a new ignition system, novel configurations for point heating and modular heating stations, a design method and a portfolio of patents.

Impact

A VIP event for selected senior managers in industry was hosted at the UK Moscow Embassy (https://www.gov.uk/government/world-location-news/global-leaders-in-russia-meet-on-energy-efficiency-sustainable-environment). A Brainstorming Event for mid-level technical R&D managers was held in Moscow. The UNIHEAT 1st and 2nd Annual Conferences were held in Moscow (http://www.uniheat-project.com/news/uniheat-hosts-inaugural-annual-conference)and St. Petersburg (http://www.uniheat-project.com/news/uniheat%E2%80%99s-second-annual-conference-23rd-october-2014-st-petersburg). Dissemination events were held in Moscow, Dubai, Hannover and Houston, and a further set is planned. A presentation of the project to the Institution of Chemical Engineers (IChemE) was broadcasted live on a webinar to a vast international audience.

The UNIHEAT project was featured in a keynote presentation titled "The technical edge: how science and technology will transform the way we find, produce and use energy" (session on "The role of innovation and technology in shaping the oil and gas industry") by David Eyton, BP's Group Head of Technology, at the World Petroleum Congress in Moscow in June 2014. As of June 2014 a total of 1690 visits were recorded to the project website (http://www.uniheat-project.com) by 975 unique visitors with > 42% returning to the site and over 5 pages per-visit.

Industry Workshops with individual companies were held with Weatherford, Schlumberger, Shell, Sibur, Sibur-Niost, Lukoil and others, generating a number of testing projects and MOUs. A day in London and a special Workshop in Novosibirsk in April 2014 were dedicated to preparing for Technology Transfer from the project, with participation of all academic leaders, the IEP team and senior personnel of Imperial Innovations and their counterparts at BIC. A technology audit and commercialisation plans have been prepared.

We are now regularly invited to hear and participate in other Russian-UK research initiatives and are creating much international good will on the ground at a time of a big diplomatic and commercial chill (see attached)

In the first two years, 7 international and 9 Russian patents were filed, with 5-7 others in the pipeline. At present, discussions are under way with the input of Imperial Innovations for launching 3 Spinoff companies.

International standing

All members have top international reputations in the field (for profs **Macchietto** & **Matar** see Team section): **Prof. G Hewitt** published >500 papers and books in multiphase flow systems and heat transfer. Wide experience of industr. applic. as founder/manager, Heat Transfer and Fluid Flow Service (HTFS) at Harwell + extensive consulting. Member, Royal Acad. of Eng. (1985), Royal Soc. (1990), and US Nat. Acad. of Eng. (1998). Awards include Donald Q. Kern Award by AIChE (1981), Max Jakob Award by ASME (1995), Luikov Medal by ICHMT (1997) and Global Energy Prize, World Economic Forum (2007). **Prof. G Jackson** is a recognised authority in the molecular description of matter and prediction of properties of dense fluids and materials. Developed highly accurate equation of state for the thermodynamic properties of complex fluid mixtures, SAFT-VR, with extensions to polymers, electrolytes, and inhomogeneous systems underway. International reputation in modelling of liquid crystals. Several highly-cited papers, including one of the most cited of the last 30 years according to the American Chem. Soc.'s Ind. & Eng. Chemistry Res. J. **Prof. S Kazarian** develops & applies advanced vibrational spectroscopic and chemical imaging methods, including ATR-FTIR spectroscopic imaging and confocal and tip-enhanced Raman microscopy. Widely recognised for his work & industrial applications in polymers, biological systems, forensics & crude oil analysis. Editorial board, Vibrational

Spectroscopy, assoc. editor, Applied Spectroscopy. Awards include Abbott Volwiler Donation Award for res. in Pharmac. Sciences, 2007; Rector's Research Excellence Award, ICL, 2007; Advanced Grant, The European Research Council, 2008; 350th Anniversary Summer Science Exhibition, The Royal Soc. , 2010. Fellow, Soc. for Appl. Spectrosc. & Royal Soc. of Chemistry. **Dr. C Markides** researches high resolution (optical laser-based) techniques for the measurement of fluids; Efficient conversion and utilization of low grade heat and 'total energy' integration; Thermodynamics of and heat transfer effects in unsteady devices, machines and heat exchangers. Awards include: 3 Outstanding Paper Awards at HEFAT2014 for Best Papers in Turbulence; Multiphase Flows; and Applications. Outstanding Paper Award at HEFAT2012 for Best Paper in Thermodynamics. Young Scientist Award for Best Quality Paper, 8th Intern. Conf. of Comput. Methods in Sciences and Eng., 2010; John Winbolt Prize for Best Journal Paper, U. of Cambridge, 2005. **Dr. M Millan-Agorio** research focuses on Catalytic upgrading of heavy oil and coal-derived hydrocarbons; Characterisation of fuels and carbonaceous materials in terms of their molecular weights and chemical structures; Thermochemical processing of solid fuels such as coal, biomass and wastes. 2004 Townend Prize, Dept. of Chem. Eng. ICL, for his PhD work. **Prof. E Muller** research focuses on: Molecular simulation of complex fluids adsorption & interfacial phenomena; Phase equilibria & thermophysical properties bridging size scales from atomistic simulations to equation of state modelling; application to engineering & environmental problems & high performance computing for engineering. Fellow, Royal Soc. of Chemistry, 2011; Editorial Board, Molecular Simulation; Executive Committee, Thomas Young Centre for Theory and Simulation of Materials, 2010; Advisory Board, Adsorption Science and Technology. **Dr. F Coletti**, co-founder & CTO of Hexxcell Ltd., is UNIHEAT 's Industry Engagement Manager. Interests in modelling, optimisation & integration of energy systems. 2010 Newitt prize for theoret. and computatl. excellence, Dept of Chem. Eng. for his PhD thesis. 2 years as Development Specialist in Cryogenic Systems R&D group, Praxair Inc., USA. Co-authored >15 j. articles & refereed conf. proceedings; co-edited monograph on Crude Oil Fouling (Elsevier, 2015); Exec. Editor,Heat Exchanger Design Handbook, the standard reference on heat transfer, heat exchangers & assoc. technologies.

Beneficial effects

The project brought together complementary competences within Chem Eng and with the Boreskov Institute (arguably one of the best in catalysis worldwide), generating excellent scientific results, excellent new personal and institutional contacts and a reserve of goodwill that will long outlast the project.

The scientific output has been abundant and very exciting, with long term impact potential, e.g.:

- the experimental characterisation of crude oil & blends (where complementary equipment, approaches and tests on the same oils have been highly revealing)
- the prediction of crude oil properties utilizing a variety of techniques, from molecular simulation to equations of state (where validation against some of the experimental structure data for asphaltenes, the use of synthetic "model" compounds, and integration with CFD and plant scale simulation are particular achievements)
- the accurate measurement of crude oil thermal fouling at various scales, from nano to refinery scale heat exchanger conditions, using the same oils.
- the development of models for deposition of inorganic as well as organic material and effects on thermo-hydraulic performance and cleaning of heat exchangers and pre-heat trains
- the complete development, from initial idea to full concept and a patent portfolio, of a new technology for catalytic heating of pipelines and industrial heating.

The team concluded that, just at Imperial, it has a worldwide unique set of multidisciplinary capabilities to offer (theoretical, computational, experimental) in an area of very high scientific and industrial interest, and the demonstrated ability to effectively integrate them towards the solution of big problems. The team are now

actively discussing the formation of a new Centre, so as to retain these unique capabilities, make them visible and offer them to industry for large scale projects.

The project has provided an excellent demonstration, and ample international visibility, of the College's ability and ambition to carry out excellent research and take it all the way to demonstration and technology transfer in a planned, actively managed and joined up way , what Prof. Macchietto , the project PI, calls "Innovation by Design". A key component is the provision of a well-designed Industry Engagement Programme, including adequate finances, dedicated professional manpower and integrated management with the Research Programme. The close collaboration with and involvement throughout by Imperial Consultants (ICON) and Imperial Innovations is particularly acknowledged as a success factor. This may represent a useful model for future projects. The college has enjoyed excellent international visibility from project presentations at key international conferences (both specialised and general) and participation in many industrial conferences, workshops and exhibitions throughout the world (Europe, Russia, Middle East, USA).

UNIHEAT opened up new visibility and opportunities in a region (Russia) which was new and quite difficult for the College. It demonstrated the ability to make a complex international project work and generated excellent goodwill in terms of international diplomacy (both in UK and Russia). The college team members are regularly invited as Speakers by various Russian (and international) organisations.

Successful funding of a number of related and follow-up projects include: **BP** (Muller et al): Total £497K on 2 projects on Coarse-grained simulation of Asphaltene Phase behaviour and equation of state development" and "Carbonaceous deposits modelling of Asphaltenes". **EU FP7** (Markides): £1.2M (£210k to IC) Grant (FP7-SME-2013/BSG-SME/605826) on 'Innovative High Efficiency Phase Change Fluid Based Heat Engine (Up-THERM)';

Discussions are under way on a number of new industry projects arising directly from the UNIHEAT work (e.g. novel flow metering technologies, fouling in plate heat exchangers, grey-water waste heat recovery), as well as 3 spinoff opportunities.

Nominator Comments

We are delighted to support the Uniheat project team for this award. They are an excellent fit to the criteria, first and foremost demonstrating a strong combination of excellence in fundamentals and industrial and societal relevance. The programme is a genuine international collaboration and the team has taken on a significant challenge in engaging in an unfamiliar geography; their success in this particular endeavour is to be lauded. An interesting feature of the programme is the very broad range of disciplines involved, covering most of the research themes in our Department. The programme has helped to foster enduring collaborations between investigators in the Department that have opened up new opportunities and helped identify new challenges to address. The number of high quality outcomes is very impressive and the benefits to both the Department and the external collaborators equates to many multiples of the investment. We recommend the team very highly for this award.