Institution: University of Birmingham

Unit of Assessment: : UoA 12 - Aeronautical, Mechanical, Chemical and Manufacturing Engineering (Chemical Engineering submission)

Title of case study: Positron emission particle tracking (PEPT) enables a paradigm shift in process design and multi-scale modelling.

1. Summary of the impact

The technique of positron emission particle tracking (PEPT), conceived and developed by David Parker from the School of Physics and colleagues in the School Chemical Engineering, has enabled a paradigm shift in the understanding of a number of industry relevant chemical engineering problems. The ability to interrogate the motion of fluids and particles within opaque systems has led to its adoption across a wide range of industry sectors including oil and chemical, minerals, and home and personal care leading to improved process models. Key process improvements have been reported by six major industrial sponsors, representing significant fiscal benefit, environmental benefits and enhanced competitiveness.

In addition to a continuing programme of studies at Birmingham, PEPT measurements are now performed at the iThemba National Lab in South Africa, where since 2009 a PEPT facility has been developed with assistance from Parker and funding from AngloAmericanPlatinum.

2. Underpinning research

PEPT was conceived and developed at the University of Birmingham as a tool for studying the fundamentals of flow in physics and engineering. PEPT is a variant of the medical imaging technique positron emission tomography (PET). Both rely on detecting the pairs of back-to-back gamma-rays emitted during positron/electron annihilation as a first step to localising a positron-emitting radioactive tracer, but whereas in PET the concentration of a radioactively-labelled fluid tracer is mapped in 3D, in PEPT a single radioactively-labelled particle is accurately tracked at high velocity. This makes the technique much more suitable for studying high speed flows. The technique can be used to study flow in granular material (by labelling and tracking a single grain) or viscous fluid flow (using a neutrally-buoyant tracer particle). As the gamma-rays concerned are highly penetrating, measurements can be made through thick steel walls, enabling non-invasive studies to be performed on realistic engineering systems involving opaque multiple phases.

The basic concept was first described in the paper by Parker (Professor of Physics) *et al.* in 1993[3.1] and the technique has been continuously developed and refined by the Birmingham group in the subsequent years through the development of improved positron cameras, tracer labelling techniques and methods for extracting information from the PEPT data.

In 1999 the original Birmingham positron camera (initially developed for performing PET studies) was replaced by a commercially-available gamma camera PET system leading to a dramatic improvement in sensitivity and precision of location in PEPT[3.2].

Since 2001, the PEPT Centre has been underpinned by EPSRC Platform funding joint with Chemical Engineering involving Dr Bakalis (Reader) and Professors Barigou, Fryer, Seville (all Professors of Chemical Engineering) as co-Investigators. This has enabled the capabilities of PEPT to be extended by adaptation of redundant medical PET scanners as transportable modular positron cameras, allowing PEPT measurements to be performed on larger-scale equipment and off site on process plant[3.3].

Other critical developments are significantly higher data rates and accurate tracking of faster-moving tracers. Early studies were restricted to labelling and tracking glass spheres of several mm in diameter, but thanks to a continuous programme of research and development a wide range of materials with sizes as small as 50 μm can now be labelled and tracked. The radionuclides needed for this work are produced using a cyclotron: to this end in 2002 the elderly Radial Ridge Cyclotron was replaced by the MC40 Cyclotron, funded by EPSRC (Co-I Seville) which enables production of a much wider range of positron-emitting radionuclides.

In parallel with these developments, techniques have been developed for extracting information such as time-averaged velocity fields and dispersion coefficients from the PEPT data. This has enabled a wider range of chemical engineering problems to be examined, including multiphase flows in equipment relevant to the oil and chemical[3.4], minerals[3.5], and home and personal care industries[3.6].

3. References to the research. Outputs 3.4, 3.5 and 3.6 best indicate research quality

3.1 Positron emission particle tracking - a technique for studying flow within engineering equipment, D J Parker, C J Broadbent, P Fowles, M R Hawkesworth and P A McNeil Nucl. Instrum. & Meth. **A326** (1993) 592-607 (can be supplied on request to the HEI)

3.2 Positron emission particle tracking using the new Birmingham positron camera, D J Parker, R N Forster, P Fowles and P S Takhar, Nucl. Instrum. & Methods **A477** (2002) 540-545, DOI: 10.1016/S0168-9002(01)01919-2

3.3 Characterisation of the latest Birmingham modular positron camera, T W Leadbeater, D J Parker and J F Gargiuli, Measurement Science and Technology **22** (2011) Article no 104017, DOI: 10.1088/0957-0233/22/10/104017.

3.4 Hydrodynamic measurements of up- and down-pumping pitched-blade turbines in gassed, agitated vessels, using positron emission particle tracking R P Fishwick, J M Winterbottom, D J Parker, X F Fan, E H Stitt, Ind. Eng. Chem. Res. **44** (2005) 6371-6380, DOI: 10.1021/ie049191v.

3.5 Positron emission particle tracking as a method to map the movement of particles in the pulp and froth phases, K. Waters, N. Rowson, X. Fan, D. Parker, and J. Cilliers, Minerals Engineering, **21** (2008) 877-882, DOI: 10.1016/j.mineng.2008.02.007.

3.6 Dynamics of textile motion in a domestic washing machine C MacNamara, A Gabriele, C Amador, S Bakalis, Chem Eng Sci, **75** (2012) 14-27, DOI:10.1016/j.ces.2012.03.009.

4. Details of the impact

Prior to PEPT, much of the understanding and optimisation of industrial processes was performed via mathematical modelling without the crucial ability to experimentally validate the models. PEPT is the only existing technique capable of imagining complex flow, mixing and comminution (grinding) processes within opaque industrial equipment. Optimisation of these leads to minimisation of processing time, enhanced throughput and in the case of mineral processing a reduction of wear on expensive plant. The revolutionary development of the PEPT has permitted both the validation and further refinement of process modelling and has been widely used within the industrial processing sector. Companies such as AstraZeneca, Johnson Matthey Catalysts and Procter and Gamble have used the technique for optimization of processes ranging from drug manufacture to understanding washing machines and dishwashers – leading to cost and efficiency savings. In the mineral sector, the technique has been used by Xstrata and AngloAmerican Platinum to reduce wear of key components in their extensive production plant. The following paragraphs describe how the work of the PEPT Centre has led to impact within a range of industrial processes and sectors during the current REF census period.

Refinement of industrial polymer extrusion[5.1]: PEPT has been used in an investigation of polymer flow and mixing behaviour within industrial twin-screw processes via an EU funded project, called PEPTFlow[5.1]. This project ran until December 2009 and had a significant impact on the competitiveness of European SMEs throughout the polymer supply chain, realising higher added value and improved products and services. The project brought together 20 organisations (research groups, equipment manufacturers and industrial users).

The measurements were used to determine the influence of key parameters such as machine design, process operation and polymer system. The results were used to establish knowledge based machine design criteria and operation guidelines, and to develop both new and existing commercial simulation and modelling software – the results were applied to eight different commercial case studies. Highlights of the impact generated include improved masterbatch colour reproducibility with reduced pigment addition based upon improved screw configurations (Treffert Group Polymer-Technologie), an enhancement in the predictive capability of the “Ludovic” CFD software package developed specifically for Twin Screw Extrusion (Sciences Computers Consultants and Fraunhofer-ICT) and the optimisation of carbon nanotube utilisation in conductive polymers, leading to a fourfold reduction in electrical resistance of the product (Rosseter Holdings Ltd). (description adapted from supporting material on PEPTflow website[5.1] and CD[5.2]).

Pharmaceutical manufacture studies[5.3]: Continuous processing has recently emerged as an area of interest for the pharmaceutical industry, where potential benefits include faster and lower cost of development, increased process robustness, improved product yields and greater supply chain flexibility. Roller compaction and twin screw wet granulation are two important technologies which can be used to achieve continuous granulation.

The *roller compaction* process involves the compaction of fine powders into ribbons or flakes that are subsequently milled to produce granules. The milling process is critical for controlling the properties of the granules, but an understanding of the governing design and operating factors is still in its infancy. PEPT was employed to examine the kinematics of roll compacted ribbons at various milling speeds using both single tracer and two tracers approaches. The PEPT data revealed that the mill speed plays an important role. At low mill speeds, the milling process is dominated by cooperative motion of the ribbons and the blade, with size reduction occurring primarily by abrasion. At high mill speeds, ribbons move randomly with comminution by impact breakage. This research was funded by AstraZeneca (description adapted from supporting statement from AZ[5.3].

"The rich information that PEPT has generated ....has led us to improved granulator and process design" Formulation Sciences Group, Global R&D, AstraZeneca[5.3].

Washing machine and dishwasher design[5.4]: The work done on characterisation internal processing in mechanical washing devices has influenced the design of the cleaning formulations and has led to products that minimise energy and water usage. Procter & Gamble is one of the largest R&D employers' in the North East of England and over the last 10 years have developed a strong relationship with Birmingham University – both with Chemical Engineering and Physics. Through the use of PEPT they have been able to quantify mechanical forces within washing machines, allowing them to understand mass transfer limitations in the laundry washing process. These insights are leading to an optimisation of P&G detergent formulations and to significant improvements in energy efficiency and environmental performance. The potential is quite significant; in Europe alone, about 270 billion washing operations are performed annually, each using about 20 L of water and 1 kWh of power. In order to realise the full potential of their formulations in reducing the amount of water and energy required during cleaning, careful characterisation of the phenomena occurring during cleaning under real conditions is critical; only PEPT has been able to provide this to-date. In the short term, the use of PEPT has allowed P&G to improve the methods used to evaluate performance of formulations under real conditions, resulting in faster and cheaper testing at their technical centres. (adapted from supporting statement from P&G[5.4]).

"...use of PEPT has allowed us to improve methods to evaluate performance of our formulations under real conditions, resulting in faster and cheaper testing..." [redacted], R&D Director, P&G.[5.4]

Catalyst manufacture and development[5.5]. Johnson Matthey Catalysts have used PEPT to understand fluid mixing in liquid continuous (solid-liquid, gas-liquid) multiphase systems within stirred vessels and static mixing devices. As a measure of the importance of PEPT to its business, Johnson Matthey continue to support PEPT through five projects (three EngD and two PhD).

"The impact to the company lies in the translation of the qualitative and quantitative learning available uniquely from PEPT into improved operation and models for existing manufacture as well as acceleration in development with decreased technical risk for new processes".
[redacted], Scientific Consultant & Chief Chemical Engineer, Johnson Matthey.[5.5]

PEPT has been applied in three core areas. The first is the use of PEPT to investigate solid-liquid-gas mixing in stirred vessels has enabled measurements to be made for the first time at industrially relevant conditions for hydrogenation and oxidation reactions using heterogeneous catalysts made by JM. The step-change in understanding that this entailed has enabled improvements in reactor design and operation. The second area is in use of PEPT to obtain mixing patterns during fed batch precipitation, used to manufacture catalysts and recover precious metals – both core JM products. Simultaneous PEPT and Electrical Resistance Tomography measurements have enabled the relationship between mixing and precipitate properties to be obtained; this data has been used to improve existing processes. The third area is in the processing of dense non-Newtonian slurries which are a vital component of emission control catalyst manufacture; data obtained using PEPT have enabled chemical and physical effects due to the multiphase nature of the materials being processed to be quantified, which has led to impact in the improved design of plant to produce catalyst washcoats and precipitates; via validated mathematical process models which can now be used with confidence. Most recently, PEPT has been used to validate a DEM mathematical model of a Turbula® mixer used for powder blending which is now being applied in commercial applications. (adapted from supporting statement from Johnson Matthey[5.5])

Minerals Processing[5.6,5.7]. IMERYS, the world's largest industrial minerals producer has used the PEPT facility at University of Birmingham for a number of years to develop a better understanding of flow patterns and media behaviour in vertically stirred mills. These mills are used to reduce and control the size distribution of kaolin, calcium carbonate and fibres for the paper, paint and polymer industries. The mills are a large energy cost for the company (up to 500kW/hr per tonne of product) and mill performance optimisation can make a significant impact on plant production costs. The work carried out with PEPT has enabled 5-10% energy savings in some plants, with a 1% saving being significant to operation[5.6]. Novel understanding of the impact of the media flow patterns and key operational variables gained using PEPT have been adopted on site in the calcium carbonate and fibre businesses[5.7]. PEPT studies have

"enabled a level of product optimisation that would have not have been possible using industry-standard industry empirical approaches", [redacted], R&D Manager, IMERYS.[5.7]

Research using PEPT has resulted in the patenting of new types of grinding media by IMERYS for calcium carbonate production and the implementation of heavy media milling techniques in IMERYS European site operations[5.6]. Current research is on development of production routes using PEPT to model mill optimisation and batch/continuous feed systems for a newly patented micro-fibrillated cellulose product (FiberTech™) for the paper market using IMERYS designed vertically stirred media mills[5.7]. IMERYS have an ongoing commitment to PEPT research, funding three research students via a £400k TSB grant (adapted from statements from IMERYS).

PEPT in South Africa. The PEPT technique developed at Birmingham has now been established at iThemba Labs in Cape Town[5.8] (2009). This facility was established with key support by the Birmingham Group and mirrors Birmingham's facility. This has now led to significant impact in the mining and milling sector. The commercial nature of many of these developments mean that companies will not release details of direct economic benefit, but the annual revenue of companies such of AngloAmerican Platinum exceeds £1B and there has been significant impact on their operations from this research. Impact has been generated by the South African facility in the following areas:

Comminution in platinum mining[5.9]: A project funded by XSTRATA to use PEPT to study the wear in stirred mills used for minerals comminution in platinum mining led to mill designs with improved lining materials in critical regions.

Performance of tumbling mills[5.9]: Initially funded by the South African Minerals to Metals Research Institute, SAMMRI, the PEPT study provided insights on the influence of key design variables on mill performance and the data was used to test a simulation model. The work has attracted follow-on-funding from AngloAmerican Platinum which has enabled optimum speed, and thus energy savings to be made for various types of tumbling mills.

Optimisation of Ball Mill operation[5.9]: AngloAmerican Platinum are using PEPT to study the behaviour of charge and grinding media in laboratory-scale ball mills in order to optimise operating conditions and reduce energy consumption (typically comminution corresponds to 65-80% of energy used in the mine-milling process). A simple model of mill operation has been developed. To enable results obtained at laboratory scale to be adapted to full scale plant, AngloAmerican Platinum has recently instrumented its full scale mills with sensors for process characterisation.

5. Sources to corroborate the impact (indicative maximum of 10 references)

5.1 www.peptflow.com.
5.2 PEPTflow CD (available from HEI)
5.3 Corroborating statement from Formulation Sciences Group, Pharmaceutical Development, Global R&D, AstraZeneca.
5.4 Corroborating statement from R&D Director, Procter & Gamble , Brussels Innovation Centre.
5.5 Corroborating statement from Scientific Consultant and Chief Chemical Engineer, Johnson Matthey Catalysts.
5.6 Corroborating statement from Chemical Engineer, IMERYS Minerals.
5.7 Corroborating statement from R&D Manager, IMERYS Minerals.
5.8 Corroborating statement from Head of Department of Physics, University of Cape Town.
5.9 Corroborating statement from Head of Comminution Research, University of Cape Town.