Institution: Imperial College London

Unit of Assessment: 12 Aeronautical, Mechanical, Chemical and Manufacturing Engineering

Title of case study: 12. Process Systems Enterprise Ltd

1. Summary of the impact (indicative maximum 100 words)

Research into new process modelling tools and numerical simulation and optimisation algorithms at Imperial's Centre for Process Systems Engineering (CPSE) has resulted in a powerful new modelling technology. In 1997, a team from (CPSE) established a spin-out company, Process Systems Enterprise Ltd (PSE, www.psenterprise.com), to commercialise this process and energy systems modelling platform - gPROMS^{TM} and to provide associated leading-edge model based services such as the design of new processes and the optimisation of existing processes.

Based on turnover (£400k at launch to £10m today), PSE is now recognised as a leading provider of process modelling technology and modelling platforms, with over 100 employees in high-end jobs. Its customers include most of the world's leading chemical, energy and automotive companies (e.g. Dow Chemical, BASF, BP, Shell, ExxonMobil, Toyota, Honda, Ford, Mitsubishi Chemicals) and it has a strong international presence with offices in the UK, US, Germany, Japan and Korea and agencies in China, India, Saudi Arabia and Thailand. The overall benefit to industry over the REF period is estimated to be £400m. The software allows customers to model, understand and optimise their processes in an unprecedented manner, leading to improved designs and more efficient operations. The gPROMS^{TM} software is used in over 200 universities for both teaching and research (primarily the latter), where it enables research into new chemical and energy processes to take place.

2. Underpinning research (indicative maximum 500 words)

The UK Research Councils set up the Interdisciplinary Research Centre (IRC) in Process Systems Engineering (CPSE); it ran until 2001 with total core funding of about £20m, supplemented by a similar amount from a broad range of sources, notably a strategic research partnership with Mitsubishi Chemical Corporation. CPSE's research focussed on the development of process modelling technology and its application to process design, operations and control. Although CPSE was a joint research centre with UCL, the research leading to the gPROMS platform took place at Imperial.

The early version of the gPROMS technology was wholly developed within the CPSE, primarily funded by the IRC block grant, with the development of the modelling technology being undertaken in the period 1993 to date.

The research programmes in CPSE were organised into a number of thematic areas including:

- Process synthesis and design;
- Process operations and control;
- Process modelling and numerical methods.

In each of these areas, ground-breaking developments in modelling languages (both for process models and for operating procedures), numerical solution techniques, experimental design, dynamic optimisation, and applications to process design and operation, took place.
The research related to the innovation was in the area of modelling, simulation and optimisation of chemical and energy processes which have a combined discrete and continuous nature. A number of challenges arise in attempting to model these processes, including the need for a comprehensive model description language for such processes, and the need for describing operating procedures and solving complex, dynamic hybrid systems models. These were addressed through the development of a novel, formal modelling language and compiler derived from the design of programming languages and their compilers [1]; a language for describing process operations and operating procedures [1]; new numerical methods for discrete-continuous simulation (solution of partial differential algebraic equations with discontinuities and equation/variable switching) [3, 4]; and new algorithms for dynamic optimisation [2, 6] which exploit the particular features of process systems. This research platform was then extended to allow integration with other tools developed elsewhere [5]. The core staff involved were John Perkins

(in post 1993-2001), Costas Pantelides (in post 1993-date), Stratos Pistikopoulos (in post 1993-date), Sandro Macchietto (in post 1993-date) and Nilay Shah (in post 1993-date).

These leading-edge research activities all fed into the development of the gPROMS modelling framework. Another feature of CPSE's research programme was "major integrated projects"; these were used to integrate strands of basic research and undertake development activities in collaboration with industry, which enabled rapid evaluation on industrially-relevant problems and refinement of the methods. A significant proportion of CPSE's budget was oriented to a major project around the design and implementation of a next generation process modelling architecture, the result being the development of a prototype tool, tested with a group of potential users, based on CPSE's industrial consortium (see below) and including Unilever, ICI, Du Pont and Dow Chemical.

The basic research that underpins gPROMS resulted in two major awards: a Queen's Anniversary Award for Education (2003) and a Queen's Award for Enterprise: Innovation (2001).

3. References to the research (indicative maximum of six references)
* References that best indicate quality of underpinning research.

*[1] P.I. Barton, C.C. Pantelides, "Modeling of combined discrete/continuous processes", AICHE Journal, Vol 40, pp. 966-979, (1994) ISSN:0001-1541 DOI: 10.1002/aic.690400608

*[2] V.S. Vassiliadis, R.W.H. Sargent, C.C. Pantelides, "Solution Of A Class Of Multistage Dynamic Optimization Problems .1. Problems Without Path Constraints", Ind. Eng. Chem. Research, Vol 33, pp. 2111-2122, (1994) ISSN:0888-5885 DOI: 10.1021/ie00033a014

[3] V.D. Dimitriadis, N. Shah, C.C. Pantelides, "Modeling And Safety Verification Of Discrete/Continuous Processing Systems", AICHE Journal, Vol 43, pp. 1041-1059, (1997) ISSN:0001-1541 DOI: 10.1002/aic.690430418

[4] B.R. Keeping, C.C. Pantelides, "A Distributed Memory Parallel Algorithm For The Efficient Computation Of Sensitivities Of Differential-Algebraic Systems", Mathematics and Computers in Simulation, Vol 44, pp. 545-558, (1998) ISSN:0378-4754 DOI: 10.1016/S0378-4754(97)00099-2

* [5] F. Bezzo, S. Macchietto, C.C. Pantelides, "A General Methodology For Hybrid Multizonal/CFD Models - Part I. Theoretical Framework", Computers & Chemical Eng., Vol 28, pp. 501-511, (2004) ISSN:0098-1354 DOI: 10.1016/j.compchemeng.2003.08.004

[6] V. Sakizlis, J.D. Perkins, E.N. Pistikopoulos, "Explicit Solutions To Optimal Control Problems For Constrained Continuous-Time Linear Systems", IEE Proceedings-Control Theory and Applications, Vol 152, pp. 443-452, (2005) ISSN:1350-2379 DOI: 10.1049/ip-cta:20059041

4. Details of the impact (indicative maximum 750 words)

Developing high fidelity models is both a challenge and an opportunity for the process and energy industrial sectors. Such models allow the de-risking of new designs, facilitate scale up, and help to troubleshoot and debottleneck existing operations. The returns on investment in modelling exercises are in principle very high relative to the potential benefits. However, the development and analysis of process models is a challenging task due to the need for a high level of user skill, and the need for effective tools for model description and model solution. In 1997, Process Systems Enterprises Limited (PSE) was formed by a team of academics (Macchietto, Pantelides, Perkins, Pistikopoulos, Shah) from the CPSE to meet these challenges, and to ensure the impact of research from the CPSE.

Since 1993 CPSE has operated an industrial consortium. Member companies of this consortium (ranging in number between 8 and 12 over the years, with typical fees of £15,000 per annum) have an opportunity to evaluate software prototypes (under special licences) and provide feedback. This model of prototyping, testing and feedback proved an invaluable part of the commercialisation process. It helped to ensure that once PSE was launched, a software platform that would meet the needs of users was available. This combination of basic and industrially-oriented research,

together with strong user engagement in the research and development phase, meant that there was a queue of ready customers as soon as the commercial version of the technology was made available. Additionally Professor Costas Pantelides, who was the team leader for the R&D activities, moved from CPSE to PSE Ltd in 2000 where he continues as the Managing Director to date, while retaining a 0.4FTE position in the CPSE. Additional routes through which the impact has taken place include the provision of consultancy services by staff from the Dept to PSE, the recruitment by PSE of PhD students and research associates and the facilitation by PSE of a partnership agreement between ABB and Imperial College.

At the launch of PSE, the gPROMS^{TM} modelling platform, including modelling language, solution algorithms, results visualisation and prototype user interface, comprised an IP package that was licensed to the company by Imperial Innovations, in return for 35% of the equity. Hence the research outputs formed the core of the company's assets. The company then worked on improving the usability, developing documentation, business development and incorporating new innovations arising from CPSE. PSE Ltd has so far solely commercialised IP arising from the CPSE, and all its revenues can be traced back to the research at the CPSE. Important impact indicators for PSE Ltd include:

- A thriving company which has current annual revenue of £10m and cumulative revenues since inception of £97m (approx £40m during the REF period).
- A global presence (with offices in the UK, US, Germany, Japan and Korea, and agencies in Saudi Arabia, Dubai, Thailand, Malaysia, China and Taiwan with over 60% (on average) of revenues from outside the UK; it is therefore a key export earner[19].
- PSE employs approximately 100 people in high-end jobs.
- PSE's products are in routine use in major companies (including 7 of the world's top 10 chemical companies) and over 200 universities, and form part of industrial practice.
- PSE has an ongoing record of innovation with new products (e.g. in solids [12], offshore safety [14], and systems modelling in healthcare, including pharmacokinetics and pharmacodynamics [13]).

PSE's platform enables the easy construction and solution of first principles models with a powerful and user-friendly tool; this has made possible a variety of new approaches to model based process design and optimisation such as:

- design of a new chemical process for a Korean chemical company that saved $5m in reactor costs alone [8];
- design of a new, "cleaner" propylene oxide process [10], where the user could consider all the trade-offs across the whole process simultaneously and therefore ensure a global optimisation while implementing a process which decouples the production of propylene oxide from that of styrene. Dr Hilario Rodriguez of Repsol states *"We increased total annualised profit by several tens of millions of €/year"* [8];
- design of new integrated devices such as fuel cells [11], including effective systems engineering and design, and the consideration of issues such as water management and heat transfer, which enables the design of fuel cells which are robust to transient operation;
- design of new crystallisation processes [12], which enables tight control of particle size distribution;
- scale up of an impact mill [15], where P&G reduced risk and experimental effort through modelling;
- Optimising the production of terephthaldehyde (TPAL) [16] through multiscale modelling, resulting in much better temperature control, saving $2m-$4m per year;
- Improved life cycle service offers from a catalyst manufacturer to its clients [17], where models are used to advise the catalyst manufacturer's clients on the optimal operation of their processes.

All of the above have been undertaken by PSE's industrial clients, who are generally in the chemicals, energy and health, foods and lifestyle industries. Typically, the return on investment in modelling these applications using PSE software and consulting is at least 10 and in the case of [8] below closer to 100. **The overall impact from commercialisation of modelling tools based on research in the CPSE over the REF period is therefore around £400m, and since inception in**

1997, £1bn. The Chemical Systems Discipline Head of P&G [18] has indicated his willingness to corroborate this impact and respond to panel queries.

PSE's vision of model-based applications used throughout the process lifecycle is now being realised, with modelling supporting discovery (e.g. in pharmaceuticals [12,13]), design (across a wide range of operations) and operations (e.g. safety assessment [14]).

The impact of the commercialisation of the software from CPSE was recognised when four of the academic staff (Machietto, Pantelides, Pistikopoulos, Shah) involved in launching PSE were part of a 5 person team awarded the MacRobert Award and Prize in 2007. This is the UK's premier award for engineering innovation and recognises *"world leading engineering developments…." Which demonstrate innovation, commercial success, and benefits to the community"* [9].

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

[7] "Leading Catalyst Manufacturer Standardises on PSE Technology & Services" (2006) http://www.businesswire.com/news/home/20061106005343/en/Sud-Chemie-AG-ChoosesgPROMS (Archived at https://www.imperial.ac.uk/ref/webarchive/nrf on 5th September, 2013)

[8] "PSE process design optimisation services" http://www.psenterprise.com/consulting/whole_plant_optimisation.html (Archived at https://www.imperial.ac.uk/ref/webarchive/prf on 5th September, 2013)

[9] "Modelling moguls scoop UK's biggest innovation prize" Royal Academy of Engineering (2007) http://www.raeng.org.uk/news/releases/shownews.htm?NewsID=392 (Archived at https://www.imperial.ac.uk/ref/webarchive/qrf on 5th September, 2013)

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[12] PSE Releases Major Update of gCRYSTAL Process Modelling Software- Enhanced usability and speed for leading crystallization design and operation tool- Enhanced Online News (2012) http://eon.businesswire.com/news/eon/20121112005110/en/gcrystal/crystallization/solidsprocessing (Archived at https://www.imperial.ac.uk/ref/webarchive/rrf on 5th September, 2013)

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[14] "PSE Oil & Gas safety" Process Systems Enterprise http://www.psenterprise.com/oilandgas.html (Archived at https://www.imperial.ac.uk/ref/webarchive/trf on 5th September, 2013)

[15] "gSOLIDS user stories-P&G – A low-cost, low-risk scale-up procedure for impact mills" Process Systems Enterprise http://www.psenterprise.com/gsolids/success_stories.html (Archived at https://www.imperial.ac.uk/ref/webarchive/vrf on 5th September 2013)

[16] S.B. Shin et al, "Optimize terephthaldehyde reactor operations", Hydrocarbon Processing, 2007 (4), pg 83-90 (Link) Archived here on 29/10/2013

[17] C Baumler, Z. Urban and M.Matzopoulos, "Enhanced methods optimize ownership costs for catalysts", Hydrocarbon Processing 2007 (6) pg 71-78 (Link) Archived here 29/10/2013

[18] Chemical Systems Discipline Head, Proctor & Gamble R&D to confirm the overall impact from commercialisation of modelling tools.

[19] http://www.psenterprise.com/company.html Archived here on 29/10/2013 .