Institution:	Imperial College London
Unit of Assessment:	12 Engineering
Title of case study:	Process Systems Engineering
Period when the underpinning research was undertaken:	2000 - 2020

Details of staff conducting the underpinning research from the submitting unit

Name(s):	Role(s) (e.g. job title):	Period(s) employed:
Claire Adjiman	Professor of Chemical Engineering	1998 – present
Amparo Galindo	Professor of Physical Chemistry	2000 – present
George Jackson	Professor of Chemical Physics	1998 – present
Sandro Macchietto	Professor of Process Systems Engineering	1993 – present
Costas Pantelides	Professor of Chemical Engineering	1993 – present
Stratos Pistikopoulos	Professor of Process Systems Engineering	1993 – 2016
Nilay Shah	Professor of Process Systems Engineering	1993 – present

Period when the claimed impact occurred:	1 August 2013 – 31 December 2020
Is this case study continued from a case study submitted in 2014?	Yes

1. Summary of the impact

Research from the Centre for Process Systems Engineering (CPSE) has led to technology that accelerated digital transformation in the process industries via the CPSE spin-out Process Systems Enterprise Limited (PSE). This resulted in the following impact during the current REF period:

1) transformed PSE into a process simulation market leader since 2014, achieving annual revenue growth to more than GBP16,000,000 in 2019, with more than 160 employees world-wide, and **acquired by Siemens AG** (for an estimated sum of GBP100,000,000 or more) in 2019;
2) underpinned the enhancements to PSE's flagship product, the gPROMS™ platform, which now forms the **umbrella platform for Siemen's** process system digital portfolio;
3) supplied integrated digitalization platform for PSEs and Siemen's clients including most of the major oil, and numerous pharmaceutical, consumer products and food companies, to **maximize their economic benefits** by capturing essential process knowledge via digital twins to create value during the process lifetime;
4) generated society impact through PSE by launching the Academic Teaching Highway (PATH) initiative that **trains chemical engineers for industry** with 21st century skills, with over 200 institutions now using the gPROMS software in their training.

2. Underpinning research

The research in the Centre for Process Systems Engineering (CPSE) focuses on developing modelling technology for process design, operations, and control. Although CPSE is a joint research centre with UCL, the research leading to the gPROMS™ platform that powers PSE took place at Imperial. PSE's model-based solutions span the whole process lifecycle via this platform yielding fast, safe, and more efficient decisions through rapid and effective exploration of the decision space. The underpinning research programmes that led to the impact described in Section 4 has the following thematic areas:

- Synthesis, design, operations, and control;
- Molecular systems engineering.

Synthesis, design, operations, and control [R1-6]

In each of the areas underlying this theme, developments in modelling languages (both for process models and for operating procedures), numerical solution techniques, experiment design, dynamic optimisation, and applications to process design and operation, have taken place. In modelling, simulation and optimisation of chemical and energy processes, the

solution of partial differential algebraic equations featuring discrete and continuous variables, discontinuities and variable-switching, required the following combination of underpinning research developments:

- **A comprehensive model description language for such systems, and bespoke new numerical methods for discrete-continuous simulation** [R1,2]: this work pioneered the linking of scales via hybrid methods that maximised computational efficiency whilst building in the relevant level of Multiphysics [R1]. It also presented algorithmic frameworks for efficient explicit online control that obviated the need for repetitive solutions of online optimisation problems.
- **Efficient algorithms featuring Monte Carlo evaluation of derivative-based global sensitivity analyses** [R3]: this work also highlights the fact that optimal selection of Monte Carlo methods to maximise computational efficiency is dependent upon the problem's effective dimensionality.
- **Experiment design and assimilation of experimental data** [R4]: This work highlights the need for sound statistical tools to evaluate model quality and accuracy, the absence of which results in models that have either too few or too many parameters; these models require trimming down or enhancing before they can be used. Moreover, this work was influential in arguing for the development of bespoke models for design, control, monitoring, and optimization.

Molecular systems engineering [R5-6]

This is a formal framework for materials modelling based on the use of the Statistical Associating Fluid Theory (SAFT) equation of state, which enables powerful predictive capabilities for a range of thermodynamic and transport properties. This work is formulated within the group contribution approach, with molecules represented as comprising distinct chemical groups. It represents a step-change in the level of accuracy possible for the prediction of properties of complex mixtures of fluids in the entire range of thermodynamic conditions without the need for adjustable parameters. SAFT (and its variants) has been deployed by PSE for designing novel processes and solvents for CO2 capture, and in the power generation industries. SAFT-based high-fidelity models are also transferable to a broad range of active pharmaceutical ingredients and solvents enabling PSE to develop mechanistic model-based solutions for drug substance and product manufacture, and drug delivery in the pharma sector.

The fundamental research underpinning the impact generated by PSE has also been recognised through the following major awards for the CPSE team during the current REF period:

- Fellowship of the Royal Society for Jackson (2019)
- Fellowships of the Royal Academy of Engineering for Adjiman (2015) and Shah (2015).
- IChemE Guggenheim Medal for Jackson (2015)
- IChemE Sargent Medals for Pantelides (2016) and Shah (2019)
- AIChE Computing Practice Award for Pantelides (2019)

3. References to the research

[R1] Bezzo F, **Macchietto S**, **Pantelides CC**, "A general methodology for hybrid multizonal/CFD models - Part I. Theoretical framework", COMPUTERS & CHEMICAL ENGINEERING., Vol 28, pp. 501-511, (2004) https//doi.org/10.1016/j.compchemeng.2003.08.004

[R2] Sakizlis V, Perkins JD, **Pistikopoulos EN**, "Explicit solutions to optimal control problems for constrained continuous-time linear systems", IEE Proceedings-Control Theory and Applications, Vol 152, pp. 443-452, (2005) https://doi.org/10.1049/ip-cta:20059041

[R3] Kucherenko S, Rodriguez-Fernandez M, **Pantelides C**, **Shah N**, 2009, Monte Carlo evaluation of derivative-based global sensitivity measures, 5th International Conference

on Sensitivity Analysis of Model Output (SAMO 2007), Publisher: ELSEVIER SCI LTD, Pages: 1135-1148, ISSN: 0951-8320. https://doi.org/10.1016/j.ress.2008.05.006

[R4] Bonvin D, Georgakis C, **Pantelides CC**, Barolo M, Grover MA, Rodrigues D, Schneider R, Dochain D, 2016, Linking models and experiments, INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, Vol: 55, Pages: 6891-6903, https://doi.org/10.1021/acs.iecr.5b04801

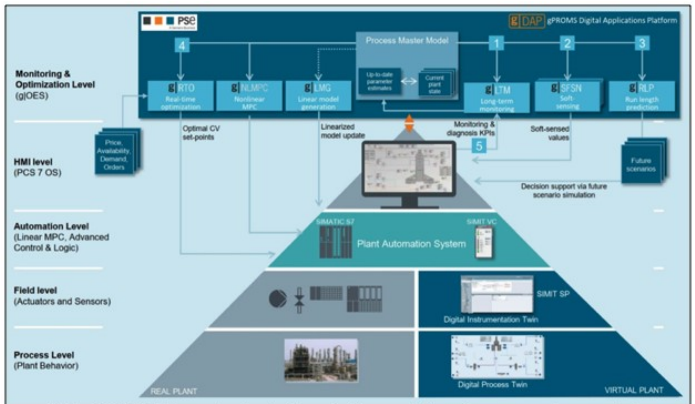
[R5] Papaioannou V, Lafitte T, Avendano C, **Adjiman CS**, **Jackson G**, Muller, EA, and **Galindo A**, 2014, Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments, JOURNAL OF CHEMICAL PHYSICS, Vol: 140, 054107. https://doi.org/10.1063/1.4851455

[R6] Lafitte T, Papaioannou V, Dufal S, **Pantelides CC**, 2017, gSAFT: Advanced physical property prediction for process modelling, 27th European Symposium on Computer-Aided Process Engineering (ESCAPE), Publisher: ELSEVIER SCIENCE BV, Pages: 1003-1008. https://doi.org/10.1016/B978-0-444-63965-3.50169-0

4. Details of the impact

The underpinning research in Section 2 has resulted in the following direct and indirect impact during the current REF period:

[I1] Directly contributed to the success of PSE: Founded in 1997 as an Imperial College spin-out by Professor Pantelides as its CEO, PSE flourished since 2014. It is now a company with over 160 employees with a global footprint (in UK, Abu Dhabi, China, Japan, Korea, Malaysia, Switzerland, Thailand, and US). Its annual turnover has grown to more than GBP16,000,000 (2019) [E1]. The contribution of our research to PSE's elevation to market leader in process simulation is clearly demonstrated in Pantelides winning The American Institute of Chemical Engineers 2019 Award with the following citation:



PSE's gPROMS is the umbrella platform for Siemens' line of process system products

> *"For pioneering work developing advanced modelling software tools (SPEEDUP and gPROMS) and transforming Process Systems Enterprise Limited (PSE) into a process simulation market leader"*. [E1]

One of the key successes of PSE in the current REF period was through partnership with, and subsequent acquisition by, Siemens AG in 2019. PSE began its collaboration with Siemens in June 2018 to develop new model-based solutions for plant performance monitoring and forecasting, soft sensing, real-time optimization, nonlinear model-predictive control and operator training based on detail process models. In October 2019, Siemens AG acquired PSE for an undisclosed sum (estimated to be "*in excess of £100m*"). [E2] According the CEO from Siemens' Process Automation Business Unit, "*PSE helps us significantly here, because now we can integrate model-based technologies from PSE in our applications in the entire plant lifecycle*." [E3] The model-based technologies from PSE is underpinned by the research conducted by our staff from CPSE.

[I2] Underpinning technical improvements in PSE and Siemens products: Our research continued to provide a technical and innovation pipeline from CPSE to PSE, contributing to enhancements to their products. The flagship product from PSE is the gPROMS™ Digital Application Platform and tools which have had several new releases since 2014. For example, in the latest release in April 2019, major enhancements included advanced

physical property prediction capabilities building on Imperial's SAFT-based thermodynamic research and powerful methods for global sensitivity analysis [E4].

Since the acquisition by Siemens, the impact of gPROMS™ has further extended due to its integration with Siemens' own digitalization portfolio for the process industry. gPROMS now forms the umbrella platform for Siemens' new series of model-based solutions (see figure). [E5]

[I3] Impact on industry: PSE's impact through the use of model-based applications throughout the process lifecycle is now being realised, with modelling supporting discovery (e.g. in pharmaceuticals), design (across a wide range of operations) and operations (e.g. safety assessment). All of the above have been undertaken by PSE's industrial clients, who are generally in the chemicals, energy, pharma, healthcare, foods and lifestyle industries. The models offered by the gPROMS™ platform allow the de-risking of new designs, facilitate scale up, and help to troubleshoot and debottleneck existing operations with a powerful and user-friendly tool; this has enabled new approaches to model-based process design and optimisation. Although the economic benefits of PSE's and Siemens' products to their industrial clients is difficult to quantify, the CEO from Siemens' Process Automation has no doubt that gPROMS™ helps to maximize the economic benefit. He stated [E5]:

> "*Equation-oriented process modelling is the specialty of gPROMS ProcessBuilder. …. The consistent application of the three digital twins for product, production and performance over the entire life cycle of a process plant* ***maximizes the economic benefit***."

Further evidence of impact of our research on industry can be found in the large number multi-national companies that use PSE products [E6]. These include:

- 5 out of 6 oil majors use gPROMS.
- The world's leading pharma, consumer products and food companies use gPROMS.
- Many of the world's most innovative companies, including leading fuel cell developers use gPROMS family products.
- 7 of the world's top 10 chemical companies use gPROMS family products.

A long list of how the gPROMS™ platform is applied to design and operational challenges in these industrial sectors can be found in [E7]. This evidence lists 42 examples in applications divided into five categories:

1) Process design (11 examples)
2) Equipment design (6 examples)
3) Process development (4 examples)
4) Process operations (17 examples)
5) Product design and development (4 examples)

To illustrate the scale and reach of the impact, here are three specific examples:

1. The design of new crystallisation processes [E8], which enables tight control of particle size distribution; scale up of an impact mill, where P&G reduced risk and experimental effort through modelling. The Chemical Systems Discipline Head of P&G has indicated his willingness to corroborate this impact and respond to panel queries.
2. Becoming a partner in the UK's Medicines Manufacturing Innovation Centre, supporting the design of continuous manufacturing innovations, where digital technologies will enable the manufacture of more personalised medicines [E9].
3. Becoming the standard solution provider for digital design and operations of a major petrochemicals manufacturer, accelerating innovation and process development [E10].

[I4] Societal impact: Educating the next generation is best conducted with tight partnership between industry and academia. In 2019, PSE launched the Academic Teaching Highway (PATH) initiative aimed at ensuring that chemical engineering graduates enter industry with 21st century skills. The PATH scheme is supported by industrial employers such as Procter & Gamble, ExxonMobil, AstraZeneca and DSM, and academic community

including Imperial. For this, PSE has become an Institution of Chemical Engineers Gold Corporate Partner, in particular for "*inspiring and developing the next generation of chemical engineers*". [E11] gPROMS is now being used by more than 200 universities for teaching and research.

5. Sources to corroborate the impact

E1 The American Institute of Chemical Engineers Awards to Prof Pantelides 2019. PDF available here.

E2 "Siemen's £100m+ purchase of PSE", 24 September 2019. https://sifted.eu/articles/siemens-pse-acquisition/ Link archived here.

E3 "Siemens Plans to Acquire Process Systems Enterprise", Mary P Bailey, Sept 16, 2019. Chemical Engineering. https://www.chemengonline.com/siemens-plans-to-acquire-process-systems-enterprise/ Link archived here.

E4 https://www.psenterprise.com/products/gproms/physprops; https://www.psenterprise.com/products/gproms/technologies/global-system-analysis Links archived here.

E5 "Partnership between Siemens and Process Systems Enterprise (PSE)". https://new.siemens.com/global/en/products/automation/industry-software/siemens-and-process-systems-enterprise.html Link archived here.

E6 PSE global client list. https://www.psenterprise.com/company/customers Link archived here.

E7 Examples of gPROMS applications. https://www.psenterprise.com/concepts/examples Link archived here.

E8 Letter from R&D VP, P&G on impact of gPROMS in their crystallisation processes.

E9 "Siemens, Perceptive Engineering and PSE become partners in the Medicines Manufacturing Innovation Centre to advance continuous manufacturing", https://www.uk-cpi.com/news/siemens-perceptive-engineering-and-pse-become-partners-in-the-medicines-manufacturing-innovation-centre-to-advance-continuous-manufacturing Link archived here.

E10 "SCG Chemicals Company chooses gPROMS modelling for digital design and operations", https://www.businesswire.com/news/home/20190322005332/en/SCG-Chemicals-Company-chooses-gPROMS-modelling-for-digital-design-and-operations Link archived here.

E11 https://www.icheme.org/about-us/press-releases/gold-standard-for-process-systems-enterprise/ Link archived here.