Institution: University of Manchester		
Unit of Assessment: 12 (Engineering)		
Title of case study: Increasing productivity in the process industries through the use of artificial intelligence and machine learning for the optimisation of distillation operations		
Period when the underpinning research was undertaken: 2003 – 2020		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Robin Smith	Professor	1984 – present
Megan Jobson	Professor	1996 – present
Nan Zhang	Senior Lecturer	2000 – present
Lluvia Ochoa-Estopier	KTP Associate	2014 – 2017
Period when the claimed impact occurred: August 2013 – July 2020		
Is this case study continued from a case study submitted in 2014? N		

1. Summary of the impact

Research into novel approaches for operational optimisation at the University of Manchester's research centre, the Centre for Process Integration, has led to increased productivity in industrial chemical processes. Operational optimisation adjusts process variables to improve the efficiency and cost effectiveness of the equipment, increasing process yields and decreasing energy use.

This research is commercially applied through a spin-out consultancy company Process Integration Ltd (PIL). The impact in this REF period has been employment of 8 additional staff, a consolidated turnover of at least GBP5,500,000, and consultancy services to more than 20 different companies worldwide. Within the impact window, the interventions detailed in this case study have resulted in client savings in excess of USD48,000,000 (GBP36,800,000).

2. Underpinning research

Complex chemical processes, such as crude oil distillation, require mathematical process models to optimise their operation in terms of key performance metrics such as process yield, energy input, and ultimately overall profitability. The complexity of these models increases with the number of adjustable parameters (inputs such as flow rates, temperatures and pressures) and the number of specifications for the different products (typically seven or more products for crude oil distillation) that must be considered. Given the associated financial and operational risks, these process models must be sufficiently accurate and computationally robust before industrial practitioners will adopt their recommendations.

Whilst conventional first-principles process models can, in principle, represent complex chemical processes with accuracy, they are mathematically much too complex for use in operational optimisation. When used in optimisation, the models may fail to converge; even if they do not fail, the optimisation cannot guarantee to give a globally optimal solution due to the highly non-linear nature of the models. For operational optimisation (whether 'off-line' or real-time), procedures need to be both robust and rapid, allowing the global optimum to be achieved with confidence.

Research at the University of Manchester (UoM) developed and applied a novel modelling approach for distillation of petroleum fractions. First, the research developed and applied a tailored machine learning-approach by using conventional detailed distillation process models to train artificial neural networks. The resulting 'surrogate' models of the petroleum refining process [1] are much simpler, much more straightforward to solve, computationally very robust and are orders of magnitude faster than conventional distillation models when applied in optimisation.

The research then incorporated previous modelling developments for existing heat recovery systems [2] to create a new method for simulation, optimisation and retrofit modification of the heat recovery system associated with the distillation process [3]. The new machine learning-based distillation modelling approach [1] was integrated with the heat-exchanger network retrofit methodology [3] and appropriate optimisation algorithms were applied. This created a novel approach for rapid, robust operational optimisation of the existing heat-integrated distillation system [4]. For example, in [4], the surrogate model used 13 neural networks to predict 89 outputs from over 20 inputs; application of the model to optimise by varying these inputs improved the profit of the heat-integrated distillation process by 130%. In collaboration with PIL, robust systematic strategies were developed for optimising the associated complex, constrained distillation systems [5]. This approach for modelling and optimisation enables process operators to carry out optimisation off-line to increase profitability of existing production facilities [6].

3. References to the research

This research is published in internationally leading journals, and is funded by an Innovate UK Knowledge Transfer Partnership project (GBP177,000). Citation counts are from Web of Science (November 2020).

[1] **Ochoa-Estopier, L.M.; Jobson, M.; Smith, R**. (2015) Optimisation of heat-integrated crude oil distillation systems. Part I: The distillation model, *Industrial & Engineering Chemistry Research* 54 (18): 4988–5000, DOI: 10.1021/ie503802j [24 citations]

[2] Rodriguez, C.; **Smith, R**., (2007), Optimisation of operating conditions for mitigating fouling in heat exchanger networks, *Chemical Engineering Research and Design*, 85 (6): 839-851 DOI: 10.1205/cherd06046 [73 citations]

[3] **Ochoa-Estopier, L.M.; Jobson,** M.; Chen, L.; Rodriguez-Forero, C.A.; **Smith, R**. (2015) Optimisation of heat-integrated crude oil distillation systems. Part II: heat exchanger network retrofit model, *Industrial & Engineering Chemistry Research* 54 (18): 5001–5017 DOI: 10.1021/ie503804u [24 citations]

[4] **Ochoa-Estopier, L.M.; Jobson, M.; Smith, R**. (2015) Optimisation of heat-integrated crude oil distillation systems. Part III: Optimisation framework, *Industrial & Engineering Chemistry Research* 54 (18): 5018–5036, DOI: 10.1021/ie503805s [14 citations]

[5] **Jobson M., Ochoa-Estopier L.,** Ibrahim D., Chen L., Gosalbez G., Li J., (2017) Feasibility bounds in operational optimization and design of crude oil distillation systems using surrogate methods, *Chemical Engineering Transactions,* 61, 1849-1854 DOI:10.3303/CET1761306 (4 citations)

[6] **Ochoa-Estopier L**.; Enriquez Gutierrez V.M.; Chen L.; Fernandez-Ortiz J.; Herrero-Soriano L.; **Jobson M**. (2018) Industrial application of surrogate models to optimise crude oil distillation units, *Chemical Engineering Transactions* 69: 289–294 DOI:10.3303/CET1869049 (6 citations)

4. Details of the impact

Pathway to impact

In 2007, Smith and Zhang established the University spin-out consultancy company, Process Integration Ltd (PIL). UMIP (now the UoM Innovation Factory) also awarded a Proof of Concept grant (GBP93,000) to Smith to develop pre-commercial software and training material, which were licensed to PIL.

PIL successfully implemented the approach developed in the research for operational optimisation of refinery distillation systems, as reported in [6]. A Knowledge Transfer Partnership supported by Innovate UK and Process Integration Ltd (2014 – 2017, GBP177,843) enabled Ochoa-Estopier to transfer the technology to PIL and further refine [5, 6] and implement novel methodologies to create software for commercial use by PIL, called i-CDU, based on [1-3][A]. During the project, PIL successfully implemented these methods for a European petroleum refinery client [6], and the KTP project was evaluated by Innovate UK as ‘outstanding’.

Reach and significance of impact

Continued growth to a global business

Based on research carried out at UoM [1–6], PIL developed and commercialised software products for different aspects of the management of physical assets. PIL focussed on the way chemical process plants operate, improving their operating efficiency to reduce energy costs and increase process yield. PIL's "*expertise and capabilities as a consultancy company are strongly underpinned by research undertaken at the University of Manchester…the root of modelling and optimisation approaches and [PIL's] in-house, and commercially available software tools, were developed based on research carried out at the University of Manchester*" [A]. PIL has reshaped their business strategy to increasingly focus on developing tools using machine learning for process optimisation and control, and continues to collaborate with the UoM including a further KTP [A].

Between August 2013 and December 2019, PIL increased its staff from 11 to 19, with their technical staff being almost all MSc and PhD graduates recruited from the Centre for Process Integration (UoM), where they gained expertise in the area of process integration [A]. The company's annual turnover has increased from GBP873,400 in 2013, to GBP1,176,100 in 2019 [A], equating to a cumulative turnover of at least GBP5,500,000 within the impact window.

PIL's service delivery has provided productivity gains to clients

Between August 2013, and July 2020, PIL have undertaken consultancy studies on 11 refinery distillation units, located in China, Spain and India [A]. Detailed below, these projects have relied upon PIL's software and consultancy capabilities (developed from the UoM research) to optimise the operation of refinery distillation units. These have led to interventions that have resulted in total client savings in excess of USD48,100,000, equivalent to a combined saving of GBP36,800,000 (November 2020):

i) In 2016, PIL undertook a consultancy project to optimise the operation of a crude oil distillation system in a European refinery. This used the i-CDU tool (developed as part of the KTP project, drawing on [1-3]) to build and apply artificial intelligence models for process optimisation. As reported in [6], the identified beneficial changes were implemented on-site, and have led to investment-free economic benefits of USD7,200,000 per annum [A] (cumulatively worth at least USD32,400,000 within the impact window).This improvement was achieved purely via operational optimisation, without any capital expenditure.

   A similar project by PIL for a Chinese refinery, improved valuable product yields with verified economic benefits of USD3,500,000 per year (USD15,700,000 in total) [A].

ii) Prior to applying the above UoM research on artificial intelligence, the ongoing collaboration with UoM and application of UoM research led to other major successes [A], as listed below. Whilst these successes were significant, the limitations encountered spurred PIL to develop new techniques based on UoM's research applying artificial intelligence:
   - Over a dozen 'Energy Optimisation Study' projects for Middle East clients have been successfully executed with a total operational saving of around USD100,000,000 per year for new design and retrofit.
   - Operational savings of more than USD3,000,000 per year were identified and implemented in steam system optimisation for a European client.
   - Operational savings of more than USD20,000,000 per year were identified and implemented in hydrogen system retrofit for a European Refinery with payback of less than 1.5 years.

5. Sources to corroborate the impact

[A] Letter of support from Chief Technical Officer, Process Integration Ltd (December 2020)