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Process Systems Engineering: Academic and Industrial Perspectives

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Abstract

In this paper, we present both academic and industrial perspectives on the research and applications of Process Systems Engineering (PSE). After a brief introduction on the history of PSE, we describe the major research accomplishments in the areas of process simulation, conceptual design and synthesis, process control, process operations and optimization. This is followed by a discussion on the industrial impact and benefits of this work, which have made it to be industrially relevant. Next, we address the issue of the current standing of PSE both in academia and in industry, and for which we present results of a survey conducted by the authors. Finally, we close with a discussion on future challenges in PSE from both the industrial and academic perspectives.

Keywords: Process systems engineering, process simulation, process synthesis, process control, scheduling and planning, mathematical programming.

1. Introduction

The field of process systems engineering (PSE) has been around in various forms for over 50 years mostly under the labels of process designs and process control. It was not until 1982 when the 1st International Symposium on Process Systems Engineering took place in Kyoto, Japan, that the term Process Systems Engineering was adopted as the general term to be applied to the different areas such as process design, control and operations, including product design.

The creation of Process Systems Engineering as a discipline can be traced back to two pioneering works. The first one is the article "Integrated Design and Optimization of Processes" published by Professor Roger Sargent in Chemical Engineering Progress (Vol. 63, Issue 9 , pp 71-78) in 1967. That article was truly visionary in that it outlined the areas of process design and integration with control and reliability, it addressed development of process models (steady state, dynamics), strategies of process calculations, and computational methods for optimization. Furthermore, the article advocated for collaborations with researchers in control systems, operations research, numerical analysis and computer science. This pioneering article outlined the future research agenda for the area of Process Systems Engineering.

The second major pioneering work was the textbok "Strategy of Process Engineering" by Professor Dale Rudd and his co-author Charles Watson, Wiley, 1968. The textbook had three major parts: a) creation and assessment of alternatives, b) optimization, c) engineering in the presence of uncertainty. The major contribution of this textbook was to present systematic approaches for each of these three topics, which nowadays are still core to process systems engineering, namely synthesis, optimization and uncertainty.

In the next section we describe some of the major accomplishments that have been achieved in Process Systems Engineering, both at the academic and at the industrial level.

2. Past accomplishments of process systems engineering

2.1. Impact in academic research

In his section we describe some of the major academic accomplishments in the major areas: process simulation, conceptual design/process synthesis, process control, process operations and optimization.

2.1.1. Process Simulation

The initial efforts in academic research in PSE were largely directed to process modeling and process simulation. The first paper on process simulators was the paper on SPEED-UP by Sargent and Westerberg (1964) at Imperial College that emphasized the ordering of computations of units in a flowsheet The concept of sequential modular simulators and its implementation was proposed by Johnson (1972) with the simulator GEMCs at McMaster University, and by Seader, Seider and Paules (1974) through their FLOWTRAN program under the CACHE organization.

The next major step was a major project funded by the Department of Energy directed by Evans, Britt, Chen, and Boston (Chen et al., 1982) at MIT and that led to the Aspen Plus simulator using the sequential modular structure, currently a major commercial simulator (Fig. 1). Next major effort took place at Imperial College through the development of gPROMS by Barton and Pantelides (1994), which in contrast to Aspen Plus adopted the equation oriented architecture. These efforts promoted the development of other commercial simulators such as CHEMCAD, Invensys, PRO-II and UNISIM. A major reference that captures the major concepts and techniques in process simulation is the book "Process Flowsheeting" by Westerberg, Hutchinson, Motard and Winter (1979).

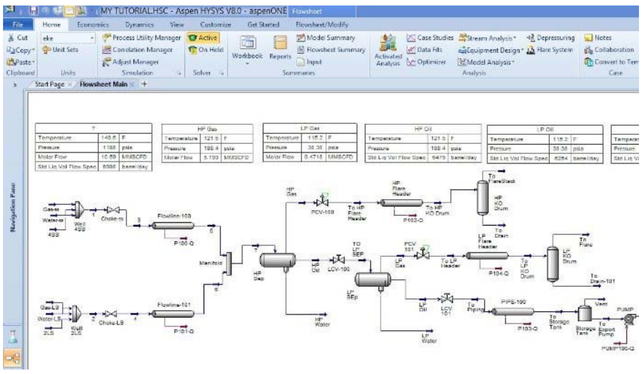

Figure 1. Simulation of a process flowsheet

2.1.2. Conceptual Design/Process Synthesis

The first textbook that was published in the area of process synthesis was the book "Process Synthesis" by Rudd, Powers and Siirola (1973). The emphasis of that book was on the generation of process flowsheets, which in turn motivated the development of the program AIDS that was motivated by initial ideas of search and problem solving in AI.

Another major development in process synthesis was the concept of pinch for heat integration that allowed the targeting of utility consumption prior to the detailed synthesis of heat exchanger networks (Fig. 2). That work was published first in the open literature by Linnhof and Flower (1978), although Ed Hohmann (1971) had previously reported a similar result. The main results were eventually published in the "User Guide on Process Integration for the Efficient Use of Energy," by Linnhoff (1994) at UMIST.

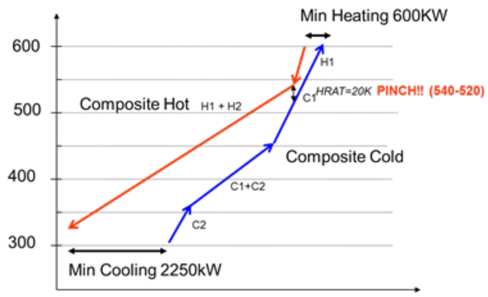

Figure 2. Pinch analysis with composite curves.

A major development was also conceptual design of process flowsheets through hierachical decomposition as proposed by Jim Douglas from the University of Massachusetts in his textbook „Conceptual Design of Processes.," (Douglas, 1988). This work together with the pinch concept motivated the work by Robin Smith at UMIST through his book „Chemical Process Design and Integration" (Smith, 2005) in which he addresses for instance the synthesis of water networks.

Finally, the concept of superstructure was first introduced by Sargent and Gaminibandara (1976) in the determination of trays in distillation columns (Fig. 3), and for which the authors modeled the problem as a nonlinear program (NLP). Subsequently, with the idea of addressing the synthesis of process flowsheets and utility plants, Grossmann and Santibanez (1980) proposed the use of mixed-integer nonlinear programming (MINLP) in which 0-1 variables are used to select potential units. These authors proposed approximations based on MILP as MINLP codes were not available at that point.

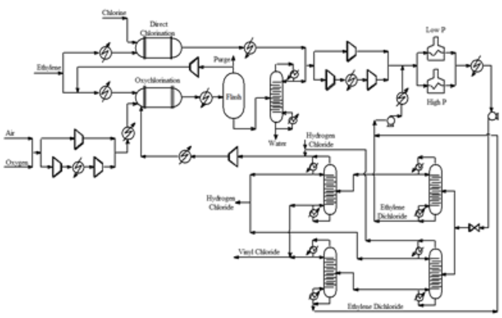

Figure 3. A superstructure for synthesizing a process flowsheet.

2.1.3. Process Control

The initial pioneers in this area were researchers like Foss (1973) at Berkeley and Luyben (1973) at Lehigh, and subsequently Shinskey (1981), whose major concern was the tuning of PID controllers. At about the same time, pioneering work on optimal control took place at Imperial College with the work by Joffee and Sargent (1973).

The next major development took place at the University of Minnesota with the work by Morari and Stephanopoulos (1980) in which they addressed the synthesis of control structures, where the major goal was to determine which variables to measure and which ones to manipulate, both at the level of units and at the level of the entire plant.

Another major step change in process control research took place with the concept of Model Predictive Control (MPC) pioneered by Cutler (1983) at his company Dynamic Matrix Control (Fig. 4). Major idea was to optimize the control actions through a receding horizon. Morari, Garcia, Prett (1989) documented some of the initial successful industrial applications of MPC, while Mayne, Rawlings, Rao and Scokaert (2000) established theoretical conditions for stability.

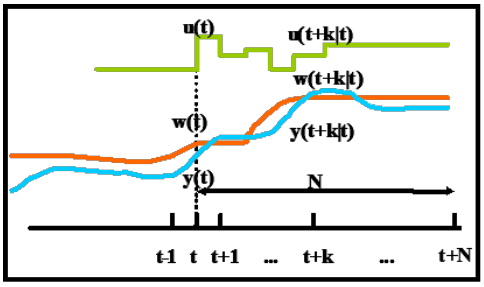

Figure 4. Model Predictive Control (MPC)

2.1.3. Process Operations

This area was not considered until the late 70's through the pioneering papers by Reklaitis (1978) at Purdue on process scheduling, and by Mauderli and Rippin (1979) at the ETH on batch scheduling motivated by the food and pharma industry in Switzerland. Espuña and Puigjaner (1989) at the Universidad Polytecnica in Barcelona were among the pioneers in applying scheduling techniques in industrial operations.

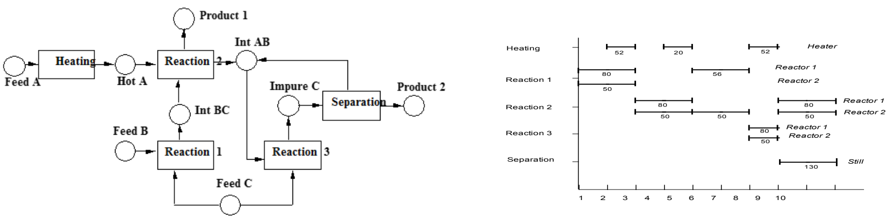

Figure 5. State-Task-Network for batch scheduling.

A major breakthrough took place at Imperial College with the work by Kondili, Pantelides and Sargent (1993) with the development of the State-Task-Network (Fig.5),. The importance of this discrete time model that is formulated as an MILP, is that it represents a very general framework that goes beyond the traditional flowshop and jobshop models used in Industrial Engineering, as it allows for complex and arbitrary network configurations.

Other important development was the area of supply chain optimization as proposed by Shah (2004) for moving away from the plant or unit level, and instead consider global process networks.

Finally, the area of operability has also emerged as another area of that is relevant for process operations. A good example is the work on flexibility and resiliency as was first presented by Grossmann and Morari (1984).

2.1.4. Optimization

Process Systems Engineering has a rich history in the area of optimization. The first branch and bound code for solving MILP problems was in fact developed by Martin Beale at British Petroleum in 1958.

The area of nonlinear programming has also been very active in PSE. The Variable-Metric Projection method by Sargent and Murtagh (1973) was one of the first methods for solving NLP problems. This subsequently motivated the development of the reduced gradient method by Murtagh and Saunders (1978) that was implemented in the code MINOS. Successive-quadratic programming developed by Han (1976) and Powell (1978) was implemented in the code SNOPT by Gill, Murray and Saunders (2005), and extended for large-scale problems by Westerberg and Berna (1980). More recent effort in this area is by Wächter, Biegler (2002) who proposed an interior-point method for NLP and implemented it in the well-known code IPOPT.

MINLP: ***Mixed-integer nonlinear programming***

$$\begin{aligned} &\min Z = f(x,y) \\ &s.t. \quad h(x,y) = 0 \\ &\qquad\;\; g(x,y) \le 0 \\ &\qquad\;\; x \in R^n, \quad y \in \{0,1\}^m \end{aligned}$$

$$f(x): R^n \to R^1, h(x): R^n \to R^m, g(x): R^n \to R^q$$

MILP: *f, h, g* linear

LP: *f, h, g* linear, only *x*

NLP: *f, h, g* nonlinear, only *x*

Figure 6. MINLP problem formulation with special cases

The next major step was in the area of mixed-integer nonlinear programming (MINLP, Fig. 6) in which Duran and Grossmann (1986) proposed the outer-approximation algorithm that was subsequently extended by Fletcher and Leyffer (1994). This method was implemented by Viswanathan and Grossmann (1990) as the computer code DICOPT.

Another important development was the extended cutting plane (ECP) by Westerlund and Pettersson (1995) that led to to code alpha-ECP.

In the area of optimization under uncertainty a first major contribution was by Reklaitis in 1975 (Friedman and Reklaitis, 1975) in the area of robust optimization for linear programming with uncertain right hand sides and matrix coefficients. This was followed by the work on flexibility summarized by Grossmann and Straub (1991) that dealt with characterizing regions of feasibility in terms of uncertain parameters and accounting for control or recourse variables that could react to the uncertainties. Subsequently the work on parametric programming by Dua and Pistikopoulos (2000) addressed the solution of various classes of mathematical optimization problems as function of uncertain parameters so that one could obtain their explicit solutions in terms of critical regions where in each of them explicit expressions for the objective function and decision variables is obtained.

The next major area that has received considerable attention by the PSE community is global optimization. For instance at Princeton Floudas and his group developed the α-BB method (Adjiman et al., 1998a; Adjiman et al. 1998b) that relied on the idea of modifying the Hessian of the Lagrangean in nonconvex NLP problems to yield a convex relaxation. The next major effort was at the University of Illinois by Ryoo and Sahinidis (1996) and Tawarlamani and Sahinidis (2002) that led to the development of the code BARON that relied on a spatial branch and bound search coupled with the use of convex underestimators in factorable functions. Kesavan, Allgor, Gatzke and Barton (2004) at MIT developed an Outer Approximation algorithm for nonconvex MINLP. Finally, Floudas and Misener (2013) developed at Princeton GLOMIQO and ANTIGONE in which a major aim was to handle bilinear terms through piecewise McCormick underestimations (Bergamini et al, 2008).

Other important efforts by the PSE community have included Logic-based Optimization at Carnegie Mellon (Raman and Grossmann, 1994), Optimal Control through orthogonal collocation at Carnegie Mellon (Cuthrell and Biegler, 1987) and integration of adjoints at Imperial College (Vassiliadis, Sargent and Pantelides, 1994), and Optimization of Hybrid Systems at Imperial College and ETH, respectively (Barton and Pantelides, 1994; Bemporad and Morari, 1999).

Finally, PSE researchers have also made major contributions in decomposition techniques, most notably Benders (1962) at Shell for decomposing large-scale MILP problems, and Stephanopoulos and Westerberg (1974) at University of Florida for Lagrangean decomposition in nonconvex NLP problems.

From the above, it is clear that researchers in Process Systems Engineering have had a major impact in the area of optimization, probably more than any other engineering discipline.

2.2. Impact in industrial practice

Process Systems Engineering research has become such a fundamental part of industrial automation and control systems that its results are often integrated into larger industrial solutions and systems and it is not anymore that trivial to recognize the role of PSE. Nevertheless, as can be anticipated based on the previous section PSE has had a remarkable impact on the way today's industry is managed. In the area of process design, e.g. energy recovery networks contribute to vast savings both from economics (USD) and environmental (CO_2) aspects, better ways to handle flowsheets and superstructures contribute both to safer and more efficient production facilities. In the area of process control model predictive control (MPC) (Garcia et al., 1989) has become a standard and most control theories and applications such as statistical process control are a result from PSE activities. In the last decades increasing attention has been given to process monitoring and fault analysis and diagnosis. In the area of process operations, almost all industrially used mathematical models for scheduling and supply chain optimization come from the PSE domain. Here, also data reconciliation and real-time optimization (RTO) (Marlin and Hrymak, 1997) have been developed closely with the oil & gas industry. As a result, many optimization and simulation tools today globally used are de facto results of process system engineering research. These include almost all algorithms aimed to solve MINLP and global optimization problems.

This is not at all a co-incidence since process system engineering has from its very early stages had both a strong focus on industrial problems, as well as, a strong interest from industrial practitioners. There have been many industrial consortia at the main PSE-focused universities, such as Carnegie Mellon University[1] (since 1985), University of Manchester[2], McMaster University[3], Imperial College[4], University of Texas at Austin and University of Wisconsin[5], to name a few. Many of these are still fully active and benefit from a membership from up to around 25 companies.

Following these facts, the PSE discipline has always been well aware of the relevant industrial problems and their significance to the practices of designing, operating and controlling complex processes. Some methodologies, however, need a strong theoretical fundament and therefore a significant research phase before being able to be deployed in the industry. A very well-known example on the design of process networks is the pinch-analysis (Linnhof and Flower, 1978). The theoretical work began in the early 70's and about a decade later the work made a big impact as it could prove 30% energy savings at chemical and petrochemical operations. After successful commercialization (Linnhoff-March) and another decade roughly 80% of all the world's largest oil and petrochemical companies were either clients or sponsors of the company. Finally KBC acquired Linnhoff-March, which was a few years later acquired by Yokogawa. This is a very common pattern, where a brilliant PSE technology is first developed and piloted in small scale but later shows such a great potential that it ends up as a central part of the product portfolio of a large automation vendor.

There are also companies that have stayed fully focused on the PSE core domain. AspenTech[6] is a good example of a company with an extremely strong PSE DNA. It started in early 80's and first focused on simulation (AspenPlus), which rapidly became

[1] http://capd.cheme.cmu.edu/

[2] https://www.ceas.manchester.ac.uk/cpi/

[3] http://macc.mcmaster.ca/

[4] https://www.imperial.ac.uk/process-systems-engineering

[5] http://twccc.che.wisc.edu/

[6] https://www.aspentech.com/en/about-aspentech/milestones-and-innovations

the most used simulator both in academia and industry. After this AspenTech has strongly extended their portfolio from refinery planning, MPC and supply chain management. This has also involved numerous acquisitions of small PSE-companies and today the AspenOne technology integrates solutions across engineering, manufacturing, asset optimization and supply chain functions. Their process information system InfoPlus.21 is one of the leading solutions in the process industries. Similarly, PSE Limited[7] was founded in the late 90's as a spin-out from Imperial College and has based its main success on gPROMS, which is today world's foremost advanced process modeling software, also used for research and teaching in over 200 universities around the world. It has also received numerous awards, e.g. the MacRobert's Award in innovation, which has been also cited as "the Nobel Prize for engineering". Multiple other success stories include the ADMC work by Charles Cutler that built the foundation of MPC, which is today a standard component of all automation vendors, as well as, ProSensus by Prof. John McGregor bringing big data analytics to the process industries already more than a decade ago. The list of similar developments is long (Haverly Systems, Chesapeake, SmartOps), not forgetting about the important developments of optimization algorithms where the PSE-community has played an important role, many of which are today available in commercial packages such as GAMS, AMPL and AIMMS.

This just highlights the fact that PSE has often contributed to future-oriented technologies, which after becoming a fundamental part of larger systems lose their PSE-roots. This is especially the case where the solution goes through multiple acquisitions and takeovers. One of the largest risk of PSE solutions is not being fully understood either technically or from their business value. The most typical setup (Fig. 7) is that a PSE group does a joint project with an industrial partner that first provides the problem requirements and some representative data for the development. Often these methodologies are not only theoretically brilliant but also proven in practice through successful pilot testing, where the collaborating company plays a key role. The main challenge occurs during hand-over (Harjunkoski et al., 2014). In order to ensure that a typical PSE solution can be taken over and maintained for years or decades, the company needs to adapt the organization such that there is a solution or product owner that can support and maintain the solution also during larger SW-migration projects. Here, the main guarantee to keep the solutions available is to make them "PhD-free", i.e. ensure that you need not be an expert to be able to manage their daily use and configuration. If it is not possible to manage the solution by the local resources, even the best solution will not survive. Unfortunately, companies do not in general anymore have optimization groups or resources driving various PSE in-house improvement projects.

[7] https://www.psenterprise.com/

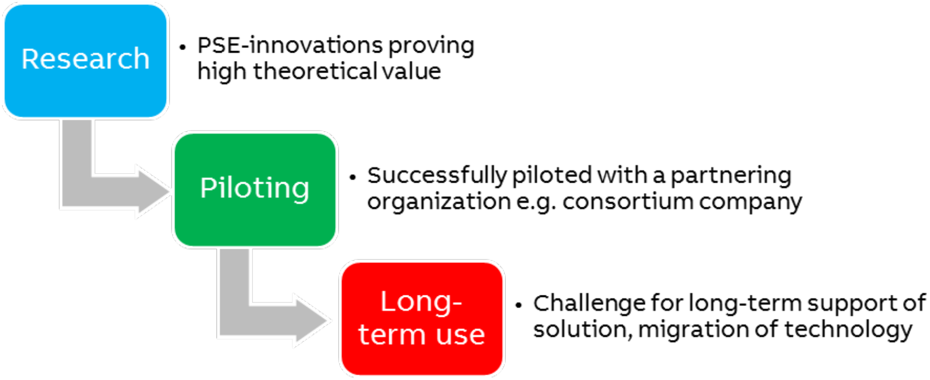

Figure 7. The path from innovation to an established industrial solution

Another major challenge apart from the lifecycle of a PSE solution is how to prove the exact value that an optimization solution contributes to the overall value chain. Often the focus is on optimizing a sub-process, which could be a control loop of a unit process, heat-exchanger network or scheduling a part of the plant. As improvements are normally continuous, the neighboring environment may also have ongoing improvement projects, both hardware as well as software focused, which makes it extremely difficult to pinpoint the exact contribution of an individual solution to the "big picture". Sometimes, neighboring solutions may even be competing against each other, e.g. when trying to increase the throughput simultaneously having another optimization solution aiming at minimizing the energy consumption and cost. Furthermore, almost no production section can work without manual interaction. Process experts frequently take the solution and modify something to match with the company practice or to avoid some safety issues that have not been considered in a model. These changes may work against the logic of an optimization solution and without clearly defined key performance indicators (KPIs) and understanding their relationship and roles it may often be impossible to tell how much an investment in a better optimization actually contributes to a better profit. To conclude, it is often crucial to analyze the entire value chain, understand the relationships between different sub-systems and focus on the overall improvement.

3. Currents standing of process systems engineering

While the area of Process Systems Engineering has been around technically since 1982 when the term was coined at the 1st International Symposium of Process Systems Engineering, the fact is that the area suffers from lack of academic recognition. Few examples to support this claim:

1. Many academics not familiar with PSE label it simply as "process control".
2. At a recent study at the National Academy of Engineering where major skill areas were identified for chemical engineering, Process Systems Engineering was not mentioned.
3. ABET, the accreditation board of engineering studies, never makes reference to Process Systems Engineering for chemical engineering studies.
4. The AIChE Division "Computing and Systems Technology Division" supposedly deals with PSE. What happened with the name of the division?
5. ESCAPE, the European meeting for PSE stands for European Symposium Computer-Aided Process Engineering (No PSE!!).

6. The flagship journal of PSE is "Computers and Chemical Engineering", again it has no reference to PSE.

The above facts motivated a survey described on the next section to gage the perception of PSE by academics as well as by industrial practitioners.

3.1. Survey results

We made a survey on the role and perception of PSE and sent it out to both academic and industrial colleagues. The questions were:

1. How many PhD and how many MSc students have you graduated in your academic career?
2. What are the major companies or universities that have hired your students?
3. Do you think your academic colleagues appreciate the importance of Process Systems Engineering?
4. Do you think industry appreciates the importance of Process Systems Engineering?
5. How do you feel about the future prospects of Process Systems Engineering in both academia and industry?
6. Do you think your company appreciates the importance of Process Systems Engineering?
7. Do you think universities attach enough importance to Process Systems Engineering?
8. How do you feel about the future prospects of Process Systems Engineering?

The questionnaire was answered by 81 attendants of which 81% were from academia and 19% from industry. The majority of the answers came from North America (62 %) and the remaining answers came from Europe (18 %), Latin America (13 %) and Asia (7 %). It turned out that the persons who responded had altogether graduated about 1200 PhD students and 1120 MSc students, i.e. more than 2300 persons in the area of PSE. This is a significant number and proved that the survey results should represent a relevant part of the community.

The list of companies and universities were vast and cannot be repeated here. It can only be said that apart from traditional process industries many graduates have also found their ways to banking / finance, manufacturing industry, as well as, pure software companies. There are also a significant number of graduates who have chosen an academic career in all major continents. The responses on the remaining questions 3-8 are shown in Table 1.

Table 1. Responses on the questionnaire

Question	Yes / positive	Somewhat / neutral	No / negative
3	42,4 %	43,9 %	13,6 %
4	57,6 %	40,9 %	1,5 %
5	71,2 %	16,7 %	12,1 %
6	68,8 %	31,2 %	0 %
7	6,2 %	43,8 %	50 %
8	81,3 %	12,5 %	6,2 %

The results show concretely that the appreciation of PSE is clearly higher in the industry than in the academia, which can also be expected taking into account the long-term synergies with industry (Fig. 8). As the challenges – both on the theoretical and practical

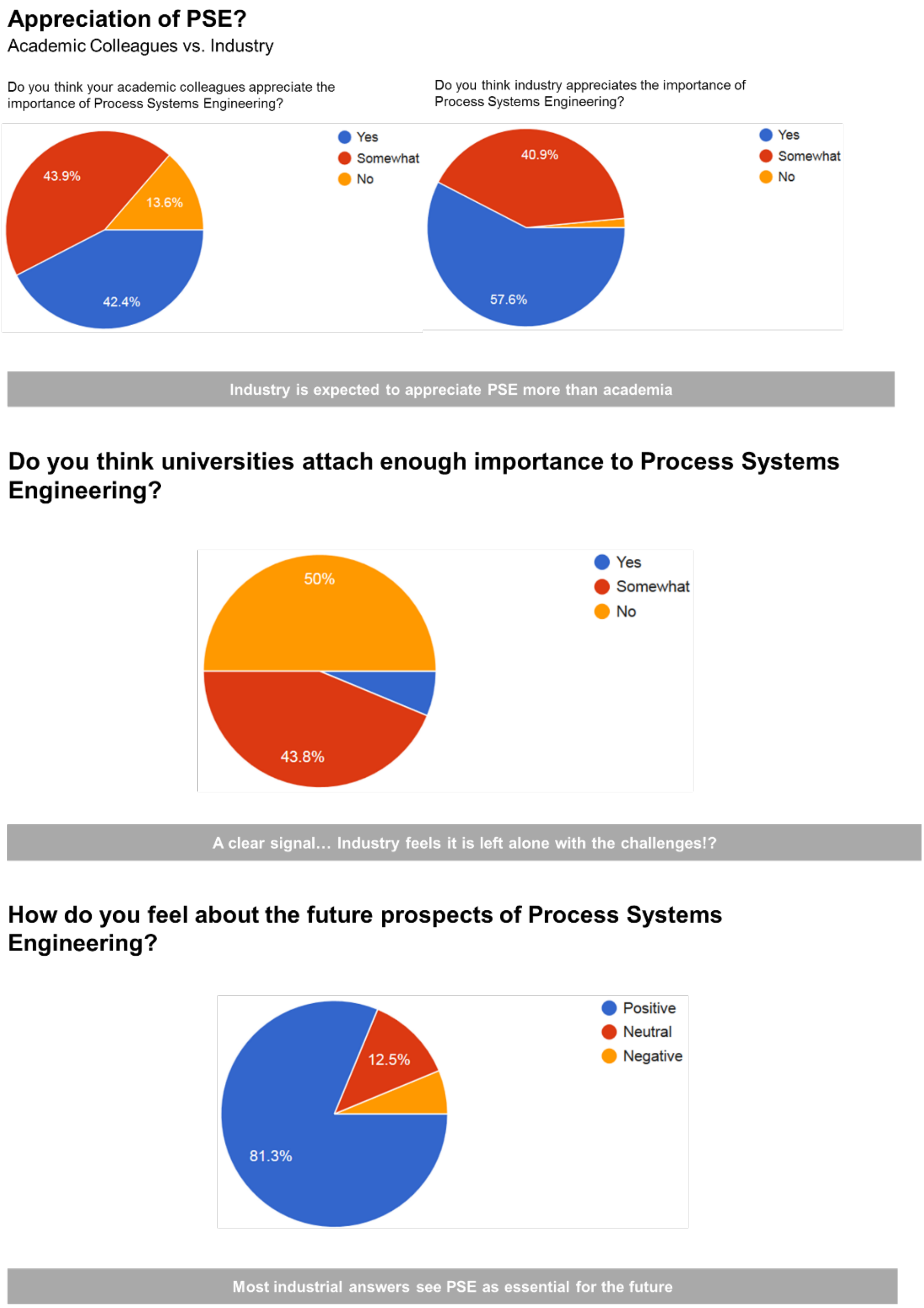

Figure 8. Some results of PSE survey.

level are increasing, most people were very positive about the future prospects of PSE. The appreciation of PSE in industry was very high and did not get any negative replies. However, the most alarming signal was that industry feels that academia is not investing enough efforts into PSE, leaving them often alone to face the current and future challenges. At the same time, industry also had a most positive opinion on the future prospects of PSE, mainly due to the numerous emerging challenges e.g. renewable energy, digitalization, including Smart Manufacturing and Industry 4.0, both of which call for more software-centric operations and control technologies. Simultaneously, exactly this fact was seen as the major threat for PSE. If the field is not sufficiently well supported by engineers and domain experts, it may be that SW-companies such as Google, Microsoft and Amazon take over part of the traditional responsibilities of PSE. It was also seen that the current view on PSE is not the same in the industry and academia, which would call for more interactions and joint coordination. Frequently there have been complaints that academia does not get access to realistic industrial problem data, as well as, industry does not have a chance to test novel appearing methods early enough. Maybe it is now a good time to join and solve these issues!

4. Future trends and major challenges in process systems engineering

4.1. Industrial Perspective

The main question is how will a process be controlled and operated in the future? Will the traditional control room operators be replaced by SW-agents? Is the level of, for instance, autonomy increasing? Will the importance of optimization increase?

On the one hand, there are driving megatrends, such as aging workforce (baby boom generation is retiring) and infrastructure (many plants were built in the 70's), shift in consumer patterns (more individualized products), environmental concerns (climate change and global warming) and skills gap (there are very few people still working that know how to build a plant). These are challenges that call for more training, interactions between generations and maintaining the first principle knowledge.

On the other hand, the disruption especially in digital technologies is significant and the main focus is slowly shifting from business-to-consumers (mobile phone apps, entertainment, banking) to business-to-business apps. Here technologies such as machine learning, big data, time sensitive networking, blockchains, cloud computing, and 5G-communication are being introduced sometimes even with partially unrealistic hopes. Nevertheless, this has opened great opportunities for software vendors and almost every larger SW-company (e.g. Google, Amazon, Microsoft, IBM) is now offering platforms that can be used to host process data analytics, partially also trusting in that machine learning (ML) technologies can at least partially replace domain expertise. This is surely true especially for routine tasks but as ML mainly builds on existing training data, it is an open question how reliably it would be able to handle unexpected and new situations that never occurred in the history. Upcoming trends can also be observed in daily technology news, which report an increasing use of open source software[8], need for standardized components, companies building up strategic directions for the digitalization and cases where traditionally isolated problems are mixed and solved together. Software companies

[8] https://www.openapc.com/

also approach the process industries[9] with the aim of proving their capabilities in process analytics and decision making.

Without doubts, if the current trend continues digitalization will play a central role in forming the future operations. Here, the above enabling technologies will be creatively mixed and matched in order to provide collaborative value generation. This is truly moving towards implementing enterprise-wide optimization in practice and due to this transition there are also many threats that occur and the impact of which no-one completely understands yet. One of the major threats is cyber security. Through digitalization the amount of connected software is increasing exponentially and this may make earlier completely isolated entities vulnerable. One of the ways to estimate and avoid some potential caveats is to look at industries that are much higher up on the so called digital s-curve. These are especially financing, insurance, media and ICT businesses. Banking for instance has been possible already for more than two decades on a home PC and new security concepts are developed and introduced even today. It seems very realistic that much of that infrastructure can be modified to be used in process industries.

The motivation for digitalization of manufacturing operations is very similar to those of traditional PSE efforts: To connect different parts of the processes and increase production throughput, product quality, process yield, equipment and energy utilization and uptime, as well as, improve regulatory compliance. This should happen simultaneously while decreasing inventory, lead times, regulatory costs, waste, process and product variations & errors, cycle times, changeover times and maintenance cost. In principle nothing new, but this time these should happen simultaneously faster and in a much more holistic manner as before. This is a golden opportunity for process systems engineering!

The evolution is very visible in digital equipment. Many earlier “dummy” components are today enhanced by monitoring capabilities and connectivity. Systems are becoming faster to integrate through flexible configuration tools and more standardized interfaces. Power systems is a good example on this, especially when looking at the development of micro-grids and virtual power plants. In larger process systems, asset management has become more intelligent and many equipment are aware of their states and can estimate their remaining life time before necessary maintenance. This, combined with real-time control and monitoring, allows to combine short and long-term planning with maintenance ensuring that the productivity of a plant can be driven to a maximum.

The challenge for companies comes from the disruption[10]. How to ensure that the existing process can continue to produce and a business does not go bankrupt after too high investments and unrealistic payback times? Some guidelines are to:

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[9] https://www.repsol.com/en/press-room/press-releases/repsol-and-google-cloud-optimize-refinery-management.cshtml

[10] https://www.flowcontrolnetwork.com/6-critical-issues-manufacturers-will-face-2016/

- Ensure step-by-step introduction of internet of things concepts (protect the investments)
- IoT and new services shall not risk current production (keep production system stable also during disruption)
- Ensure transparent and controllable plant upgrades (requires also good control of data flows)
- Use standards to deploy the full and long-term potential of digitalization (where possible)
- Keep data protection and data integrity high on the agenda (consider different aspects of cyber security)

Systems become more complex as the increasing number of individual components also become more complex. This calls for flexible and adaptable design, not only of processes but also of process systems. Operations aim at 100% availability, which calls for collaborative optimization models. Simultaneously, these systems are expected to be easy to manage and configure (compare it to an iPhone) in order to maximize the operator effectiveness, as well as, reduce the needed number of highly trained individuals to fight against the competence gap. Figure 9 shows these aspects and emphasize the need for identifying and supporting synergies. This also calls for a strong collaboration between wide set of skills. The thought that the PSE-community can handle this alone is unrealistic, as we already today are building most of our work on software platforms partially designed by other domains.

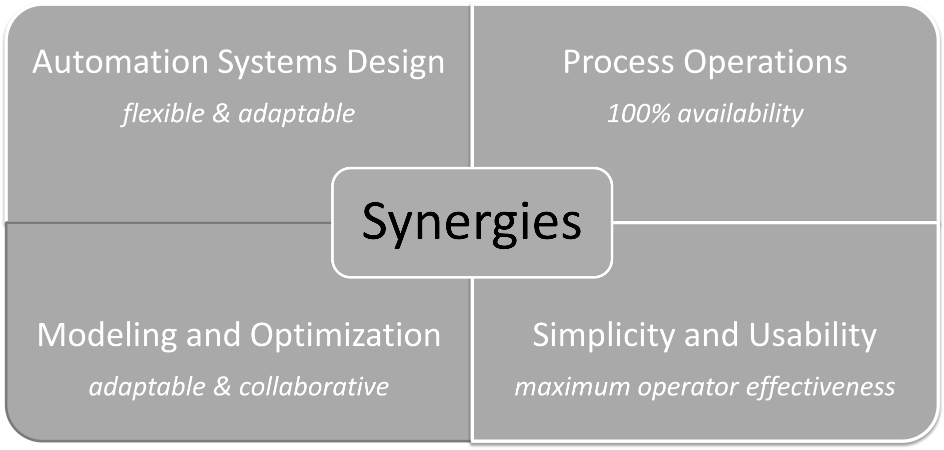

Figure 9. Synergies between the traditional PSE areas

Industries have started a journey driven by environmental awareness, governmental regulation and global competition that will most likely continue with a continuously increasing speed. Concepts such as food-energy-water nexus have not yet been considered other than on a very small scale but these types of aspects will evidently lead to a stronger regulation and dependency on external factors. The PSE community should also evaluate and adopt the best and most suitable SW-tools and platforms in order to be able to keep the pace of evolution. Research should not anymore be categorized as “industrial” or “academic” but rather by its role in a longer time scale. Novel solutions should be per design easily adaptable and early tested in industry to both evaluate their capability, as well as, raise new relevant questions in moving the digitalization and PSE jointly forward to a successful direction.

4.2. Academic Perspective

While there have been many important research accomplishments in Process Systems Engineering as discussed in section 2.1, it is clear that a number of major challenges remain in the areas listed below, and for which we provide several representative examples of on-going research to reinforce the point that research in Process Systems Engineering remains a vibrant area.

4.2.1. Mathematical Optimization. Here a major challenge continues to be the effective solution of MINLP problems. One direction has been to expand the capabilities of MINLP algorithms as has been the case of incorporating quadratic cuts in the outer-approximation algorithm (Su et al., 2018). A promising direction is the one by Ruth Misener's group (Mistry et al., 2018) who is exploring the use of Satisfability Modulo Theories that have originated in Computer Science and which have shown to provide promising results in some scheduling problems. Another important challenge are Decomposition Methods (Benders and Lagrangean) for Global Optimization under Uncertainty, which has been addressed for instance by Paul Barton and his group (Li et al., 2012). A related problem is the global optimization of multilevel optimization problems that are being addressed by Alexander Mitsos through discretization and relaxation techniques (Mitsos et al., 2008; Mitsos et al. 2010)

4.2.2. Machine Learning. This is an area closely related to optimization as has been shown by Sahinidis and his group (Cozad et al., 2014; Wilson and Sahinidis, 2017) with the development of the system ALAMO that allows the selection of a rich set of functions through the use of global optimization techniques for MINLP like BARON. A related issue in machine learning is the development of hybrid models that combine basic physical principles with data driven models based on neural networks as described by Venkatasubramanian (2019).

4.2.3. Process and Product Design. A major direction in process design has been the incorporation of molecular design for the simultaneous design of materials such as solvents and a corresponding process. Claire Adjiman and her group have been developing mathematical models based on combinatorial search and optimization to accomplish this objective. On a related effort Gani and co-workers have been developing ProCAPD, a chemical product design simulator, based on computer-aided methods for design-analysis of single molecular products (solvents, refrigerants, etc.); mixtures-blends (gasoline, jet-fuel, lubricants); and liquid formulated products (cosmetics, detergents, paints, insect repellents). As for process synthesis Chen et al. (2018) are developing superstructure optimization methods for process flowsheets using Generalized Disjunctive Programming algorithms in Python combined with global optimization methods. Major research efforts are also being undertaken by large research groups such as the RAPID project of AIChE for process intensification (RAPID, 2018) and the IDAES project lead by NETL (IDAES, 2018).

4.2.4. Planning, scheduling, Enterprise-wide optimization.. Major directions include embedding inventory policies in the optimization of supply chain planning, as described in the work by Grossmann and his group (Brunaud and Grossmann, 2017). Refining optimization continues to be relevant problem as shown by Ierapetritou and co-workers with her work on simultaneous scheduling of production units and blending (Shah et al., 2010). Demand side management has also emerged as an interesting area for scheduling the operation of power intensive processes to take advantage of changes of hourly electricity pricing, which inturn translates into improving the grid performance as discussed by Zhang and Grossmann (2016). Another interesting direction has been the development of MILP-based online scheduling as economic MPC as proposed by Christos Maravelias and Jim Rawlings who have applied this tool to the control of HVAC systems in commercial buildings (Risbeck et al, 2017). Finally, reinforcement learning has been proposed by Lee for integrating planning and scheduling in process systems (Badgwell et al, 2018, Shin and Lee, 2019).

4.2.4. Energy and Sustainability. Energy and sustainability have emerged as areas of great interest in Process Systems Engineering. A new application has been the design and operation of infrastructure for shale gas production that involves both design decisions (selection of pipeline and compressors) and planning decisions (drilling and water supply) giving rise to large scale MINLP models as described in Cafaro and Grossmann (2014) and Drouven and Grossmann (2016). Another area that has received significant attention is design of supply chains and processes for biofuels for which MILP models have been proposed as described in the work by Yue et. al (2014). Integrated solar energy with production processes has also been addressed through a systems viewpoint as proposed by Gencer and Agrawal (2017). Also, long-term planning of electric power systems comprising coal, gas, nuclear, solar and wind sources is also being addressed through very large scale-MILP models as proposed by Lara et al. (2018). Finally, in order to assess the environmental impact through life-cycle analysis, pioneered by Azapagic (1999), is now being expanded to sustainability issues like climate change mitigation (Galan-Martin et al. (2018).

4.2.5 Healthcare. This area, which traditionally has not been an area of focus for Process Systems Engineering, is starting to receives some attention by researchers in PSE. An example is the work by David Bogle who has been addressing the modeling of the liver as a flowsheet in order to predict 'ultradian' oscillations in the concentration of glucose produced by the liver (Ashworth et al., 2016). Another example is the work by Reklaitis to reduce adverse effect of drugs for individualized medicine for which Bayesian inference methods are combined with stochastic programming models (Jayachandran et al., 2015; Reklaitis, 2017).

5. Conclusions

In this paper, we have presented academic and industrial perspectives on the research and applications of Process Systems Engineering (PSE). We have shown that there have been major research accomplishments in the areas of process simulation, conceptual design and synthesis, process control, process operations and optimization, which in turn have translated into industrially useful methodologies and software tools. We have also shown the disconnect between academia and industry in regards to the appreciation of Process Systems Engineering. The encouraging result has been that both industry and academic researchers in PSE are optimistic about the future of the area. Finally, we have discussed some future challenges in PSE from both the industrial and academic perspectives, which will hopefully motivate the younger generation of researchers and practitioners to keep Process Systems Engineering a vibrant research area that is industrially relevant.

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