A Survey of Optimal Process Design Capabilities and Practices in the Chemical and Petrochemical Industries

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Abstract

To examine industrial capabilities and practices in using process design optimization software tools, we conducted a series of over one hundred interviews with practitioners and industry experts in optimal process design, focusing on current techniques, workflows, and challenges. In this article, we analyze the findings of these interviews, providing a perspective into the status of optimal process design in the petrochemical and chemical industries. We present the findings first separated by company type and personnel function, followed by industry-specific insights.

keywords: Optimal Process Design, Process Synthesis, Process Engineering, Process Simulation

1 Introduction

With increased competitive and regulatory pressures, the petrochemical and chemical industries strive to improve economic performance, increase energy efficiency, and lower the environmental impact of production facilities, often aided by computational tools for process modeling, simulation, and optimization[1]. In addition, many (petro)chemical products are manufactured in large quantities and sold at relatively low margins, further emphasizing the importance of effective design and operational optimization of large-scale production plants[2]. As a result, *process design* and the post-commissioning activities through which engineers continuously improve the operations of chemical production facilities are viewed as key elements of chemical engineering practice[3].

Through the various stages of process design and development, computational packages, known as *process simulators*, are used to model candidate flowsheet configurations[4], which are often highly integrated to improve efficiency and profitability[5]. Here, *modeling* refers to defining the material and energy balances for a given flowsheet structure, along with the requisite constitutive relations, and *simulation* covers the (numerical) approaches taken to solve the aforementioned balance equations. Furthermore, *optimization* techniques can be applied

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to improve process designs at various stages: at the *conceptual* level, the optimal flowsheet is selected from a superstructure (typically based on shortcut/approximate representations of unit operations), while *detailed* design entails selecting the unit specifications (column staging, reactor dimensions) and operating conditions (pressures, temperatures, flow rates, compositions) for a given, fixed flowsheet structure, in which unit operations are described in as much detail as possible. The objective functions used in optimization calculations often capture both the capital and operating expenditures associated with a given flowsheet.

The petrochemical and chemical industries began developing simulation tools for individual unit operations in the middle-1950s[6], and, while limited in number, successful use of early simulation tools demonstrated important savings[4;7;8]. Initially, many companies developed and maintained their own proprietary simulation tools. While offering the benefit of fostering deep in-house expertise and retaining complete control over the source code, such tools are typically hard to maintain (particularly when transitioning between computational platforms and programming languages) and require dedicated software engineering departments in addition to the engineers who use them. The latter disadvantages have provided the impetus for the development of general process simulators by specialized commercial entities, an effort that gained momentum in the 1980s and continues to date. Through the years, computerized process simulators have become accepted tools for engineering educators and practitioners alike[3;4], especially at (large) companies able to invest into the purchase, deployment, documentation, and maintenance of a commercial, third-party process simulation software.

The process systems engineering research community has given significant attention to advancing capabilities for large-scale process optimization[9;10], and some of the existing commercial process simulation packages now offer deterministic optimization capabilities. Nevertheless, in many practical situations, process design optimization remains an empirical effort consisting of a (guided) trial-and-error search by an experienced engineer. When performed, computational optimization is often carried out with simplified process models or as a piecewise optimization of the flowsheet[3]. Existing literature[4;9;11;12;13;14] suggests several potential causes for this discrepancy between research advances, commercial software capabilities, and the situation in practice:

- a lack of clarity concerning when the application of rigorous optimization techniques is appropriate and/or beneficial: uncertainty in system parameters (e.g., physical properties) and/or equipment cost can diminish the practical use of the results of deterministic optimization calculations, particularly at the early stages of conceptual design

- problem definition: the choice of decision variables and constraints is not immediately obvious for a new process and requires expert input even in the case of a more established plant design

- setup and computational time are difficult to predict and may be difficult to accommodate when tight project execution timelines are imposed. These issues are directly related to the robustness of numerical algorithms and their ability to deal with, e.g., algebraic loops and highly nonlinear, poorly conditioned systems of equations for which a feasible initial guess is difficult to find.

Motivated by the above, we carried out a cross-industry survey of practitioners involved in the area of optimal process design. With the goal of identifying the current status quo and ongoing challenges in this field, we conducted over one hundred interviews focusing on current industrial practice, including design project workflows, techniques and approaches, and the associated issues perceived by workers at different experience levels and in different corporate roles.

In this paper we report our aggregate findings, which we strove to make company- and technology-agnostic. We begin with our working definition for optimal process design, our initial assumptions, and the interview methodology. We then present general findings from our interviews broken down by function, insights specific to particular (petro)chemicals industries, and overarching conclusions. While we believe that our interviewee cohort represents a broad cross-section of the industrial sectors of interest, we note that the conclusions of this work result from the opinions of and challenges encountered by the interviewed individuals and may not necessarily reflect the status of the entire industry. The findings reveal a very broad spectrum of optimization use among industries, beginning with the fact that personnel in different industries have vastly different interpretations of the notion of "optimization" and the consequent wide variation in practical applications of computer-aided process optimization tools. We focused on industries that use mainly continuous processes, as they rely on a common set of tools and principles for steady-state process design. We deliberately excluded batch processing, such as the food processing, pharmaceutical, and formulated products industries.

2 Optimal process design practice: background and description of the study approach

2.1 Problem definition

When creating and evaluating a new (petro)chemical process concept, the best design must be carefully selected from multiple candidate process configurations. Research in this area, termed *process synthesis*, has converged towards representing the candidates as a comprehensive superstructure, with the expectation that the optimal structure is contained within and can be identified via a (mixed-integer) optimization procedure. Many methods have been proposed for systematic generation and optimization of flowsheet superstructures[15], and several industrial success stories demonstrate the large potential benefits of process synthesis techniques[16].

Although considerable developments have been made in optimization and computational capabilities, most methods for optimization-based process synthesis still rely on heuristics and/or decomposition techniques, whereby subsystems of the flowsheet (e.g., heat exchanger networks, distillation systems, reactor networks) are optimized separately[5;17;18]. When the full flowsheet is considered, it is impractical, except for simple processes featuring a small number of unit operations, to use detailed and nonlinear process unit models[5], and, as a consequence, optimization-based synthesis problems in the literature are typically formulated as mixed-integer linear programs (MILPs). The interested reader is referred to Chen and Grossmann (2017)[18] for more details on recent progress in *process synthesis* techniques and current challenges, given that this topic was outside the scope of our survey.

For the candidate process configuration(s) selected at the *synthesis* stage, engineers use detailed mathematical models to ensure that the optimal design is selected for manufacturing a given product palette. The mathematical models employed can vary greatly in their level of detail, and distributed-parameter models can be used to capture in more detail the relevant physical phenomena and help in identifying the equipment design decisions and process operating parameters that maximize economic efficiency[19;20]. At this stage, the impact of model accuracy increases significantly, and the development of the necessary models is often supported by pilot-scale experimentation.

We will refer to this latter step as process **design optimization**, specifically defining it as *the activity of identifying, for a fixed group of process units and connectivity structure, the steady-state process characteristics (unit sizes, stream flow rates, operating pressures, etc.) that maximize an objective function reflecting process economics while satisfying safety, quality, throughput, and regulatory targets and/or constraints.*

It is worth noting that, in addition to synthesis and design, optimization tools are also used for *control* applications in the petrochemical and chemical industries (most notably for model predictive control – MPC). The interested reviewer is referred to Qin and Badgwell (2003)[21] and Badgwell and Qin (2015)[22] for perspectives on industrial use of MPC, since, again, this topic was outside the scope of our survey.

2.2 Software tools for process design

Design optimization, as well as post-commissioning operation, can benefit considerably from the use of modern gradient-based optimization algorithms and their software implementations[23;12], yet the deployment of modern optimization algorithms in commercial and practical applications is still relatively limited[1;24;25]. From a mathematical perspective, steady-state flowsheet simulation requires solving the material and energy balances of the process units, as well as the physical property correlations or equation(s) of state for the chemical components present. The corresponding systems of algebraic equations (for steady-state process models) are often high-dimensional and typically highly nonlinear, ill-conditioned, and poorly structured[9].

Most commercial and industrial process flowsheet simulation tools use a sequential modular (SM) approach, simulating the interconnected unit operations (with dedicated unit operation solvers) in a process by "tearing" recycle streams and solving individual unit operations in sequence. The recycle streams are then converged in an interative manner by updating the simulation inputs until some convergence criterion is reached. While such SM approaches can solve process flowsheets with poor initial guesses, they are relegated to estimating gradients and sensitivities through finite difference calculations, which can be computationally expensive and potentially inaccurate[9;26].

An alternative way to simulate process flowsheets, referred to as the equation oriented (EO) approach, is to solve all of the linear and/or nonlinear model equations simultaneously[10]. The EO approach allows for custom unit operation models to be easily incorporated (since no separate solver is required) and simplifies process optimization by allowing for gradient matricies to be calculated via automatic or symbolic differentiation[10;19;27]. Despite these advantages, EO modeling environments generally rely on Newton-type solvers and require informed initial guesses to solve process flowsheet models successfully and reliably[5].

Several flowsheet simulation packages use a "hybrid" approach in order to combine the optimization-related benefits of EO process simulators and the robustness of SM process simulators[1]. These hybrid approaches typically are capable of calculating Jacobian and Hessian matrices via automatic differentiation and use SM simulation concepts to provide the informed initial guesses to initialize process models, which can require significant computational effort, particularly when the flowsheet is complex. Various numerical methods have been proposed to expedite the identification of good initial guesses and to provide alternatives to the Newton class of methods, including: 1) homotopy continuation[28;29], 2) pseudo-transient continuation[1;19;27], 3) interval Newton methods[30;31], and 4) global-optimization-based methods[32], among others.

2.3 Initial assumption and approach of the study

A relatively recent survey[33] of industrial practitioners in the systems and control area reported that respondents ranked "optimization of a process or operation" as the most important skill for chemical engineering graduates. As a result, this study was based on the assumption that process design optimization tools are needed, implemented, and used –to varying extents– throughout the lifecycle of a process, including 1) research and development, 2) engineering and construction, and 3) execution and operation (Figure 1).

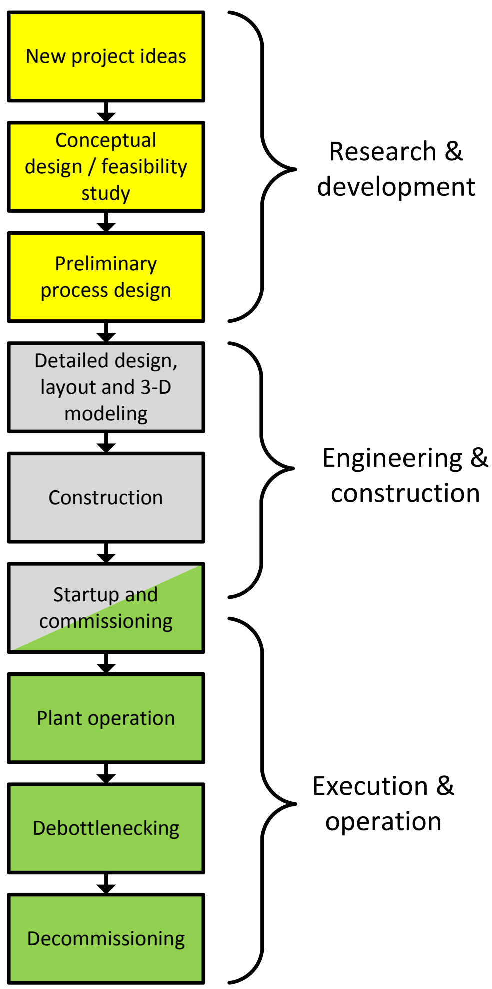

Figure 1: Typical lifecycle of a (petro)chemical manufacturing process.

To investigate the validity of this assumption, we conducted interviews with practitioners and experts working in the various stages of the process lifecycle. The interviews ranged from thirty minutes to an hour in length and were mostly conducted in-person, with a few over the telephone or video conference. The interviews were focused on participants from the United States and Canada, with a few interviewees from Europe. With the goal of identifying current optimal process design practices and challenges, we focused our questions on the interviewees' daily responsibilities, workflows, problem-solving techniques and use of computational tools, and we strove to identify challenges within each category.

In total, 110 interviews were conducted. The roles of the employees interviewed ranged from plant production engineers to process design specialists and to senior management, and interviewees were selected from various industries (base chemicals – commodity, specialty and polymers, air separation, and oil refining). A breakdown of the interviewees by roles and industrial sectors is shown in Figure 2.

The results we report below are distilled from our interviewees' responses, and as such our discussion is admittedly less quantitative than it would be had we used formal and standardized polling mechanisms (e.g., surveys). Nevertheless, we believe that this approach allowed us to truly focus the interviews on the use of optimization techniques (in their various guises and interpretations) and obtain insights that a "one-size-fits-all" questionnaire may not fully reveal.

3 Findings (I): General workflow for process design

The lifecycle of a (petro)chemical process (Figure 1) can be translated into functions and activities that belong to three main categories. Each functional category is typically the perogative of a specialized commercial entity:

- Technology licensing companies develop new process technologies, such as new catalysts, reactors, or processing alternatives, providing opportunities for the construction of new manufacturing plants or for capital improvements to existing plants. Such companies are also typically involved in the conceptual design of processes using their new technologies.

- Engineering, procurement, and construction (EPC) companies can aid in the conceptual design, and they specialize in the detailed engineering work and "putting metal on the ground", or physically installing the designed plant.

- Operating companies cover the capital investment and assume responsibility for plant operation, maintenance, and improvements until it is decommissioned.

The analysis presented in this paper generally follows this division of labor between technology development/licensing companies, EPC firms, and operating companies; however, we note that the ecosystem of the petrochemical and chemical industries is more complex. Although many companies predominately carry out one of these specialized roles, larger companies may carry out more than one of these activities in-house via separate, dedicated teams or divisions. For instance, larger EPC firms can have groups researching new process technologies that they can then license and build, or larger operating companies can have process design experts focusing on new plant development. Still larger companies may perform all three functions in-house. The implementation of new technology ideas into physical production facilities is a capital-intensive process that is managed via complex and

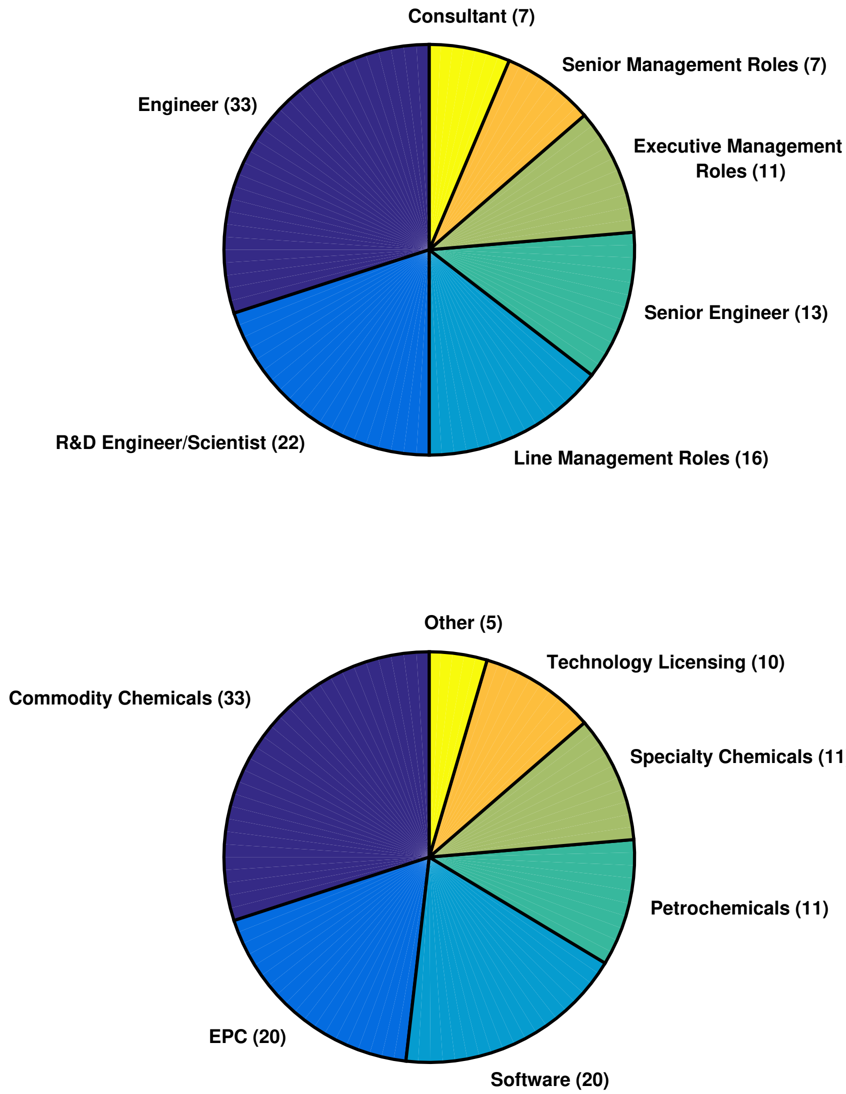

Figure 2: Structure of interviewee cohort by role in their respective organizations (top) and industrial sector (bottom).

detailed contractual agreements and supporting organizational structures, particularly when the three functions mentioned above are performed by different corporate entities. With the segregation of work and expertise along the process lifecycle among different commercial entities, the value added in each step is different for each entity in the ecosystem and results in complex interactions, manifest, e.g., in the (lack of) exchange of information and intellectual property transfer.

3.1 Process research and development

New process technologies, such as new equipment concepts or new catalysts, are often developed by companies that specialize in licensing such technologies and derive most of their revenue from accumulating licensable patents/intellectual property and maintaining valuable trade secrets. Our interviews revealed that the biggest challenge such technology developers and licensors face is that the petrochemical and chemical industries are generally very risk-averse and slow to change. It is therefore difficult to convince a potential licensee company to be the first adopter of a new technology; many personnel in our interviewee cohort emphasized the existence of a "race to be second," whereby there is a distinct reluctance on the part of technology operators to be the first to adopt a new and potentially unproven technology. Conversely, the same operators were eager to rapidly deploy *before* their direct competitors new technologies that had been *already proven by another early adopter*. We found this pattern to be most prevalent in the refining industry, where low (often single-digit) profit margins limit the amount of risk that management is willing to take. Interviewees engaged in work further downstream, such as in specialty chemicals, revealed a slightly less risk-averse attitude.

In addition to the crucial role that technological maturity plays, the main factors involved in successfully licensing a technology are capital and operating costs (CAPEX and OPEX) against yield and product quality, motivating technology licensing companies to optimize total revenue. However, this effort must strike a balance between potential per-unit cost reductions and the increased risk associated with altering a process. Experimental data surrounding new technologies are often very limited due to the fact that pilot testing is costly and time-consuming. Consequently, many of our interviewees believed that the mathematical models used for process optimization are not capable of predicting process behavior when many variables are changed, and they therefore seek to improve the process by solely focusing on the largest contributors to throughput, CAPEX, and OPEX. Management and engineers in technology licensing companies often use a divide-and-conquer strategy, where "tornado" charts (Figure 3) serve to identify the most significant revenue and cost components of a new technology. On the basis of such charts, engineers utilize the most influential degrees of freedom to maximize profit. This activity is carried out either by manually testing various scenarios (spanning design options and operating cases) or by using a computational process optimization package.

Our interviews also revealed information "silos" that prevent the use of process optimization tools, particularly by technology licensees. While often limited, pilot plant data can be (and are) used to build detailed mathematical models for at least parts of a process (e.g., the main reactor). We found that these models are typically only used internally by the technology developer company and rarely shared with potential licensees in open form; rather, a "black box" model is provided along with the design-and-build blueprint. Operating companies are thus often forced to create their own versions of the high-fidelity, "digital twin" models used internally by the technology licensor, employing dedicated equipment modeling teams to reconcile historical operating data. In addition to the considerable cost involved with effort duplication, this state of affairs represents an impediment in the consistent application of optimization strategies at the unit and plant levels throughout the lifecycle of a process.

Interviewees from all three types of commercial entities emphasized that their companies have adapted and/or developed standardized workflows for evolving a new process technology from concept to construction. These workflows share many similarities to the Stage-Gate® approach[34;35] for new product development and commercialization and involve a series of

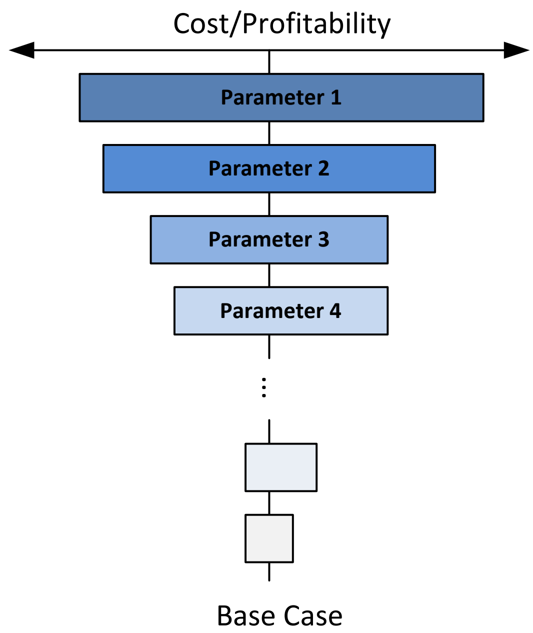

Figure 3: "Tornado" diagram for visualizing project cost sensitivities to various parameters.

stages involving project work and data analysis, each followed by a "gate". Each such gate results in a go/no-go decision concerning the continuation of the project[35], and each subsequent stage is designed to gather further information and reduce key uncertainties about a technology. It is typical that later stages are longer in duration and more capital intensive that the initial stages, which are dedicated to conceptual exploration rather than detailed studies.

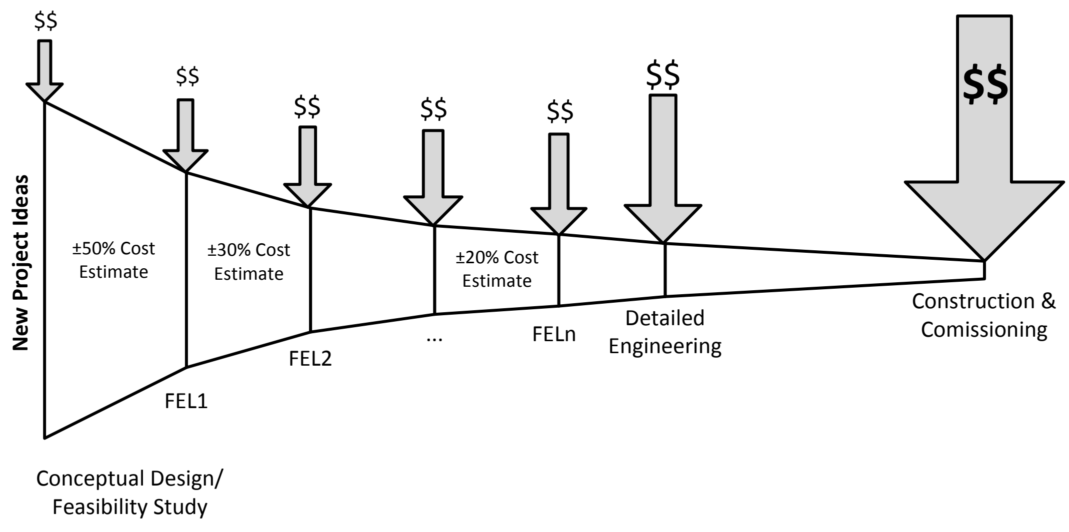

Figure 4: Workflow for process design engineering involving various stages. The arrows represent relative capital expenditures at each gate.

The initial stage in such a process adoption workflow is termed a conceptual design or feasibility study based on a new business opportunity and/or a new laboratory-scale discovery. A validated concept then progresses through a series of front-end loading (FEL) stages (sometimes referred to as front-end engineering design (FEED) or feasibility analysis), wherein designs are progressively refined and cost estimates are improved. The final stages for a new process typically involve detailed engineering – including full unit specifications, 3-D plant modeling, and relief calculations – and the ultimate decision on whether to construct the resulting designed plant.

Figure 4 shows a typical workflow for taking an idea for a new (petro)chemical process from engineering design to plant construction, as well as some of the typical levels of uncertainty at various stages. Our interactions with our interviewees revealed that in the vast majority of cases, the number of early-stage projects is considerably larger than those in the later/final stages of the pipeline. This attrition can be attributed to natural elimination of technically sound but economically suboptimal ideas (an empirical threshold of a 15% return on investment is often used), as well as to fluctuations in the type and number of business opportunities available at any given time.

3.2 Detailed engineering and construction

Once a technology has withstood the scrutiny of the feasibility study (Figure 4), it is ready for the detailed engineering design. This activity is typically undertaken by an EPC company, often in close collaboration with the operating company that will own and operate the plant. Our interviews revealed that the roles of the two entities and the distribution of labor depend on the respective levels of expertise and available manpower, ranging from complete design by the EPC to a side-by-side effort by design engineers from both the EPC and operator. The main outcomes of this design effort are, i) an accurate cost estimate for project execution, ii) a complete design blueprint for procurement and construction, and iii) a preliminary evaluation of potential project execution risks and issues. Given the high level of detail involved and the amount of domain expertise required, engineering design work is generally carried out by multiple, separate and specialized teams (focusing, e.g., on heat exchange, rotating equipment, reaction vessels, separations, piping and instrumentation, relief systems), with a well-defined central management, reporting, and interaction structure.

In the interest of accelerating the detailed design schedule and saving cost, many EPC company employees reported moving away from a "series" design workflow, in which each engineering team designs the section of the process they specialize in and passes it onto the next team, and towards a "parallel" approach, whereby the engineering teams must simultaneously complete their relevant tasks. The parallel workflow involves a block flow diagram (BFD) with heat and material balances specifying inputs and outputs for the engineering teams; the aforementioned reporting structure is used to notify of changes to these input/output values, triggered, e.g., by equipment limitations. Our interviewees noted that this workflow makes changes to the process more costly as the detailed design process advances. Given the increasingly stringent time constraints and the pressure not to make costly alterations to the process parameters, engineers tasked with carrying out detailed designs often focus on finding a solution that is feasible from the process BFD point of view, without necessarily being economically optimal (either locally at the individual block level or at the plant level).

In the particular case when only certain units or subsections of a larger process flowsheet (rather than a full plant design) are licensed from a third party, the lack of detailed model information for licensed technologies (owing to nonexistence or, as mentioned above, to the reluctance of licensors to share such models) further limits the ability of EPC and operating companies to explore a broad range of operating conditions at the detailed design and engineering stage.

EPC companies generate revenue from project execution and are keen on maintaining a robust project pipeline. Further, EPC firms are not directly vested or interested in the final operating stage of a new production facility. As a consequence, they historically tended to bill their clients on a reimbursable cost basis (charging hourly for services), ensuring that revenue is generated even when the clients' projects are stopped at an early stage/gate (Figure 4). On the other hand, the main customers of EPC firms, operating companies, are increasingly favoring lump-sum contracts, which are structured such that the EPC company guarantees a deliverable for a fixed sum and on a given schedule, assuming the financial risk if the cost exceeds the agreed-upon amount. Additional financial penalties can be imposed on schedule overruns and performance shortcomings on the delivered product.

With the growing prevalence of lump-sum contract bids, EPC companies emphasize heavily the importance of accurate capital cost estimates, enabling them to acquire projects by placing bids low enough to win business, yet high enough to guarantee the project can be completed for the price. The ability to accurately estimate equipment and installation costs is of paramount importance: management at EPC companies we interviewed reported cost-estimation teams of similar size to, or larger than their engineering teams.

As a consequence of these facts, EPC companies *very rarely perform any degree of process design optimization*, in the sense defined in Section 2. Our discussions revealed that new process BFDs typically deviate very little from proven (and often quite old) designs, with any modifications relying heavily on in-house heuristics and expertise, with the goal of maintaining feasibility and minimizing uncertainty in equipment design and cost estimates. We also found that engineers at these companies typically use spreadsheet-based tools developed in-house to create the specifications for process units, and rely on subject-matter experts for validating their decisions and for consultation in cases where the decision diverges significantly from previous solutions.

We believe that this "pattern-based" approach by EPC companies is a natural response to the high risk and capital intensive nature of the industry (and the associated risk-averse behavior of their customers), and potentially a significant contributor to the generally slow-changing nature of the petrochemical and chemical industries. EPC companies maintain a wealth of subject-matter expertise through historical records and senior experts, and they accomplish the important task of building functional, on-spec plants by relying on time-tested solutions.

3.3 Project execution and process operations

Even though technology licensing companies and EPC companies may contractually guarantee performance for (parts of) a manufacturing process, the financial risk for a new (petro)chemical plant ultimately falls on the operating company that owns it. As they directly benefit from reduced operating costs or increased throughput, many large operating companies maintain in-house process R&D teams that engage in optimal process design at the conceptual design stage (to evaluate new capital investments) and/or in process debottlenecking. Personnel in such R&D teams were generally of the opinion that commercial tools for optimal process design suffer from usability and convergence issues; using them requires significant amounts of experience and training. Further, setting up optimization problems itself takes significant expertise (to identify constraints, feasible variable ranges, etc.), so a company must invest time and effort to built up the requisite knowledge for engaging in optimal process design. The biggest challenge reported by these expert process R&D teams was model validation. The engineers are often provided with incomplete data (or data of uncertain quality) from manufacturing plants and technology licensing companies' pilot plants, making *the development of predictive models for optimization a considerable challenge*.

At the front line of such operating companies are the manufacturing plants. Relevant to this study, (petro)chemical manufacturing sites are staffed by plant managers, production engineers, and process operators. At the plant-management level, the primary concerns are ensuring regulatory compliance and safe operation, as any incidents in these areas can result in a plant shutdown and lost production. Plant managers are generally given fixed budgets each year, which they therefore first dedicate to safety- and compliance-related projects. Although not the primary concern, economic improvements are still important to plant managers, but they typically only have enough capital-improvement budget to invest in the "lowest-hanging fruit," or projects guaranteed to make the most return in the shortest time. Production engineers and process operators at (petro)chemical plants are tasked with keeping plant running smoothly, and thus spend most of their time dealing with operational issues. Although they may use computational simulation tools to identify potential issues in the plant, engineers at the plant level generally stated that *do not have the time to develop expertise in optimization tools*, as most of their efforts are dedicated to day-to-day process operations, monitoring and troubleshooting.

In the case of several operating companies, our study revealed an additional barrier for optimal process design in the interaction between engineers at the plant level and the internal R&D teams. Plant personnel often decline to implement possible improvements identified by the internal R&D teams. The latter have intimated that process engineers or operators at (petro)chemical manufacturing sites may reject a proposed change or upgrade based on factors that were not considered at the outset of the improvement initiative, including unmodeled plant behaviors such as the evolution of trace components, equipment degradation (e.g., increased fouling), or the advent of side reactions. Plant operators may also reject proposed process improvements because optimized processes are often highly integrated and/or operate very close to their bounds, making them inflexible and difficult to control. An operating point near plant equipment limits may also be more difficult to reach safely and quickly during start-up. Such outcomes can be attributed to poor project scope definition on the part of the R&D team. Ultimately, however, the responsibility of plant operators is to keep the process running as smoothly as possible, and process alterations that complicate this fundamental task are likely to not be embraced at the plant level.

The above limitations notwithstanding, our survey found that operating companies as a whole possess the most optimal process design expertise out of all three entities defined in Section 2. In addition to design optimization, many operating company R&D teams use the optimization capabilities of equation-oriented process simulation packages to facilitate the model validation process, identify debottlenecking projects, and define conceptual plant designs. The move towards lump-sum contracts between operating companies and EPC firms puts more financial responsibilty on the EPC firms, but also incentivizes EPC firms to simply build the cheapest design possible (that meets the contractual obligations). This requires that operating companies can do a sizeable amount of the conceptual and detailed design work themselves, as they must provide detailed-enough specifications to ensure the quality and performance of the design.

4 Findings (II): Industry-specific insights

In Section 3, we described our general learnings about optimal process design in the various stages of a (petro)chemical manufacturing process lifecycle. Although the value generation schemes for research and EPC firms do not vary much across different industries, operating companies in different industries face very disparate economic and technological challenges. Through our interviews, we identified several industry-specific patterns, which we relate below.

4.1 Petroleum refining

The petroleum refining industry converts the hydrocarbons in crude oil to transporation fuels, lubricants, and other products through catalytic reactions, thermal processes, separations, and blending processes[36]. The products typically have strict "macroscopic" quality specifications, such as octane number, flash properties, and/or sulfur content. Refineries may switch between different feedstock and product slates as often as daily, and the consistent quality of the end-products is typically ensured via blending. With variable process inputs and outputs, *process design is not focused on optimality at a fixed steady-state operating point*. Rather, refineries are designed to allow for flexible operation with different grades and types of raw material. The design objective is to maximize product yield and plant throughput under such circumstances; this deviates the capabilities of standard steady-state process simulation and optimization packages (which offer deterministic optimization, rather than optimization under uncertainty and/or robust optimization). We note here that engineers in refining companies did report the use of a limited number of specialized design software tools to optimize small parts of a plant, such as the design of specific reactors, or the design of a gas-treating system.

In a different vein, engineers in operating companies in the refining industries reported the extensive use of computational optimization tools at the scheduling and planning layers, aiming to determine optimal feedstock purchase and production strategies for existing plants. Fluctuating petrochemical market prices make planning and scheduling vital to maximizing profits in the refining industry. The use of real-time optimization (RTO), a steady-state optimization of the targets/setpoints of the control system, carried out periodically (e.g., every hour), is very prevalent in the refining industry[37;38]. These calculations typically involve solving a nonlinear program including pricing discontinuities, mass and energy balances, product properties, and separation thermodynamics to maximize profit or minimize cost, and practical implementation of RTO presents its own relavent challenges pertaining to imprecise economic data, model validation issues, and deviations from steady-state operation.

4.2 Commodities - air separations and chemicals

Air separation and commodity/base chemical manufacturing plants operate with relatively low profit margins. Further, especially in the air separation case, they are treated as utility suppliers by their downstream customers, with explicit expectations related to product quality and availability. Unlike the refining case, the properties of the feedstock and the product slates are relatively constant in time, allowing for *significant usage of optimal* *process design tools to maximize competitiveness*. Operating companies in these industries appear to have accumulated significant process know-how, which is captured, among others, in accurate process models. Due to the importance of process optimization, many large operating companies that manufacture commodities maintain teams of in-house process R&D experts that serve in a consulting role in optimal design projects for both new and existing plants.

Many internal process R&D teams that we interacted with at air separation and commodity chemical companies reported using equation-oriented optimization tools, with technical challenges mainly arising from difficulty of use. A special obstacle is posed by the fact that no single software tool offers all the desired features, such as equation-oriented modeling, global optimization algorithms, and simulating process start-up and failure events. Engineers are thus forced to migrate models and/or significant amounts of data between different software tools. Plant models are thus often created in multiple software packages and must be carefully cross-validated, a time-consuming and potentially error-prone process. Another reported challenge was related to presenting the optimization results and clearly defining the associated benefits, such that the probability of the solution being accepted by management is maximized.

With significant intellectual property and effort invested in commercial software tools, operating companies are often reluctant to switch software packages, but many still continually monitor new software releases to ensure they are at the forefront of technology. The required financial investment and the difficulty of using commercial optimization packages is also prohibitive to smaller companies seeking to adopt and deploy optimization techniques. As mentioned above, engineers at a company seeking to adopt computational optimization tools for the first time often find it hard to quantify the economic benefit or return on investment for using such tools. While larger companies may be willing to invest in adopting (or at least testing) new software tools, allowing them to evaluate the economic benefit directly, the limited budgets of smaller companies force them to only purchase software that is deemed essential, and (expensive) design optimization packages often to not pass this criterion.

4.3 Specialty chemicals

Companies involved in specialty chemicals production often develop new products that can be made from a limited array of (purchased) feedstock. Here, margins are high (compared to the commodities sector), and speed-to-market is of utmost importance[2]. To protect intellectual property surrounding new products, many specialty chemical companies perform the research and pilot plant functions themselves, only seeking external assistance when necessary, such as in creating the detailed design of a plant. The combination of limited knowledge about product chemistry, smaller manufacturing plant sizes, and higher profit margins leads *optimal process design to be a lower priority for most specialty chemical companies*.

To minimize time-to-market for new products, plants may be designed after only a basic exploration of the reaction chemistry or physical properties of the new compounds. Process engineers are thus facing the challenge of producing a feasible (rather than optimal) design, and the development teams often spend the bulk of their time validating physical properties for proprietary chemical components. In addition, lower production rates motivate many companies to opt for batch processes, which cannot be optimized using conventional steady-state process optimization techniques. Our interviewees reported that, if ever desired, scaling up of a specialty chemical production process poses a significant challenge due to the difficulty in predicting process behavior with a limited understanding of the chemistry and physics.

The relatively high profit margins in the specialty chemicals sector may render minimization of energy use in manufacturing a secondary concern. Additionally, the lack of full system understanding limits the potential impact of optimization tools because it is difficult to identify all of the realistic constraints on the process design. The processes are generally "optimized" by physical experimentation – changing operating points in the actual process and observing the effects. The major goals in such optimization routines for a production process in this industry are thus to maximize the production rate/throughput (often while only using existing equipment), minimizing waste generation, and meeting regulatory concerns.

5 Findings (III): Overarching trends

A recurring theme we encountered in our interviews was the difficulty in demonstrating the value of investing in optimal process design capabilities. For established processes, it is difficult to estimate the extent to which a process can be improved beyond the experience-guided, trial-and-error operational changes that were often made over the span of decades. Likewise, for new process concepts, it may be unclear how much a process can be improved based on models constructed from the limited information and experimental data available.

As a related organizational challenge, it became evident that engineers who could benefit from using optimization software seldom have the latitude to select, purchase and adopt new software tools to supplement or replace existing, established ones. This is especially true in larger companies, where the user base for incumbent tools could be quite large, and retraining this workforce would be a massive undertaking. Process R&D teams must get management approval to purchase software tools or training, but –as revealed before– such initiatives are undermined by the difficulty of quantifying the expected benefit of computer-aided optimization and calculate returns on investing in new software.

This trend was also evident in our discussion with sales and support engineers at process simulation and optimization software providers. Here, the difficulty of determining the monetary benefit of software leads to long sales cycles, often involving extensive trial periods for customers to evaluate features, added value, and product suitability to their specific needs. These companies have found that the best method for garnering interest in new software is through testimonials and case studies. Most software providers informed us that they maintain extensive case study portfolios (often including the history of adoption of the respective tool by industrial customers) that demonstrate the value of process design optimization.

A second recurring theme in our interviews was the lack of alignment in incentives and constraints among technology licensing, EPC, and operating companies. Figure 5 presents a summary of the objectives and constraints encountered by each of these entities, as well as the flow of information between them. Each entity has its own objective, and information and knowledge are compartmentalized, leading to a disconnect between those who possess detailed, predictive models (if they exist for a process) and those who would directly financially benefit from process optimization. It was apparent through our interviews that engineers at many companies felt they were building models or collecting data that a different company already had, but would not share for business reasons.

The final recurring theme from our interviews was that, aside from dedicated R&D

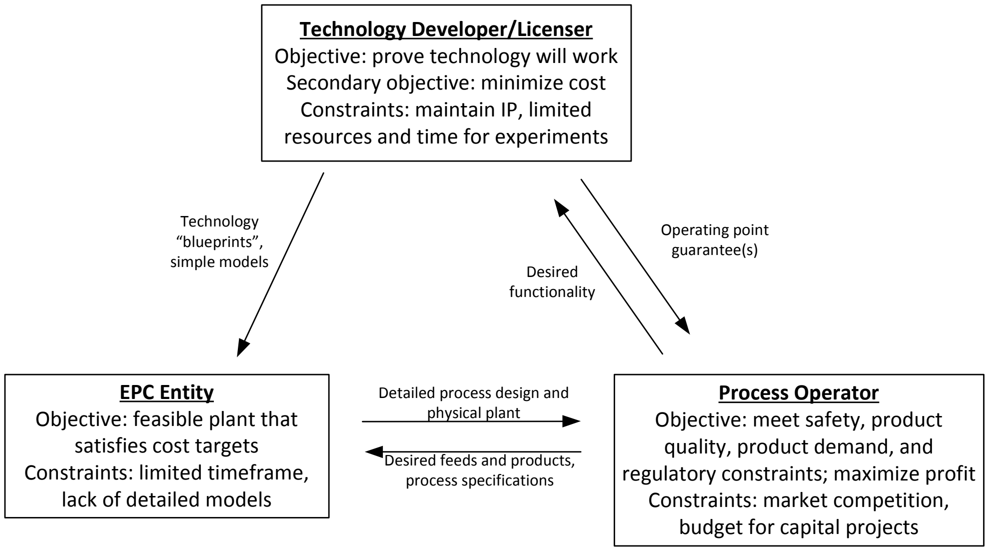

Figure 5: General objectives and constraints of entities engaged in the process design ecosystem.

scientists, employees in the petrchemical and chemical industries are cautious and hesitant to change. Owing to the magnitude of capital investments in the industry and the repercussions of safety and/or regulatory violations, the primary concern of practitioners at all levels is to ensure that processes operate reliably and predictably. There is considerable uncertainty in the design of new processes, and new operating schemes introduced by an optimization procedure – whose inner workings and decisions may not be fully transparent to the user – are often met with skepticism by plant operators, who may have an empirical understanding of the plant that goes beyond the information captured in the optimization model. Finally, the majority of our interviewees did not mention considering environmental sustainability or the entire process life-cycle beyond meeting regulatory mandates –which was mentioned extensively– when making design decisions.

6 Conclusions and perspective

Base (petro)chemicals are produced in large quantities and sold at relatively low margins, motivating research in optimal process design to maximize the economic efficiency of manufacturing plants[24;10]. Although the potential economic improvements from using large-scale, equation-oriented process optimization can be considerable, our survey of industrial experts and practioners revealed a limited penetration of such techniques into industry workflow and applications. The multitude of practical challenges faced by process engineers in their day-to-day responsibilities often preclude them from developing the requisite expertise or the predictive models involved in optimal process design.

Research companies developing new process technologies can benefit from improved economics, but the information they hold about some aspects of the process is limited and only affords a narrow window for optimization. EPC firms, which are usually responsible for the detailed design and physical construction of a plant, do not directly benefit from optimal process design and are primarily concerned with the extensive challenge of simply designing and building a plant that performs to specifications. Operating companies, who bear the financial risk of a new (petro)chemical manufacturing process, are typically the most concerned with optimal process design for cost minimization. Operating companies involved in the production of commodities are most likely to possess the process expertise and the incentive to engage in steady-state optimal process design.

Our interactions with a broad cadre of industry experts suggest that increasing the adoption of process optimization tools in practice rests on three pillars:

1. **Accessibility:** ensuring the future *seamless integration* of optimization capabilities and custom, detailed modeling in the process simulation software tools that are already familiar to industry practitioners. The implementation of optimization capabilities should target all aspects of usability: an easy to use interface for problem definition, transparent troubleshooting, fast computation and a detailed presentation and interpretation of the results. At the modeling level, the ability to deal with complex, physical models, as well as with subject matter expert knowledge (described in the form of, e.g., spreadsheets) would be very valuable. Furthermore, it is necessary to incorporate capabilities for model validation and data reconciliation, allowing engineers to minimize model uncertainty.

2. **Alignment and information availability:** sharing optimization-relevant information between the entities involved in the process design and operations ecosystem. In particular, starting at the equipment manufacturer and technology development level, each process or process concept could be accompanied by a "digital twin," a model that can be used further downstream by EPCs and operators to improve their own activities.

3. **Awareness and training:** the undergraduate chemical engineering curriculum provides limited exposure to optimization concepts (typically in the form of an elective course, which is not offered at all institutions)[33]. Graduate-level training is similarly limited[39]. As such, many engineers are not fully aware of the opportunities afforded by process optimization. Even if such awareness exists, engineers may not fully grasp the fundamentals of setting up and solving an optimization problem, recovering from solver failures and interpreting the results. Mandating that such concepts be taught at the undergraduate level is unrealistic given an already very full curriculum. A potential solution is the expansion of corporate training programs to a new model, whereby multiple companies would join forces and resources to develop the curriculum and support training of their employees. The course materials can be reasonably expected to belong to the "pre-competitive" domain, thereby ensuring that no trade secrets or valuable commercial information are disclosed. In this model, training could be provided by third party – such as an academic institution or a (consortium of) commercial software provider(s), further ensuring the "neutral" nature of the course. Employees could be incentivized to enroll in such training programs by providing, e.g., credits towards professional engineering licensure.

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