

Guidance for Developing First-of-a-Kind Projects and Processes

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New products and processes, such as critical mineral processing, alcohol-to-jet fuel, advanced plastic recycling, and battery recycling, have the potential to drive new value through performance or cost improvements targeted to evolving market needs in the oil, gas and chemical industry. To realize this value, however, organizations must navigate a challenging path through development and scale-up of first-of-a-kind processes.



Whether it is new to an organization, new to an industry, or a true first-of-its-kind innovation, a novel chemical process introduces unique challenges for project planning and execution, including unanticipated technical complexities, unknown risks, and limited existing knowledge as an early pilot design is scaled up to commercial-scale.

By aligning the right skills and employing best practices for knowledge transfer and project risk assessment, the development team can anticipate common issues, find fatal flaws quickly and generate vital insights as early as possible — when they have the greatest potential to help control costs and lay the groundwork for a successful project.

Best Practices for Guiding First-of-a-Kind Projects

First-of-a-kind projects introduce a unique concurrence of project execution and process development challenges. The engineering team may be responsible for assessing viability in the face of substantial uncertainty and before process development is complete.

Traditional project execution models are poorly suited to incorporating major changes once execution is underway. However, the development cycle for novel projects often results in a timeline where a commercial-scale project enters detailed design while process development is still ongoing. Successful commercialization will require the management team to exercise both flexibility and discipline to achieve successful startup within the constraints of a reasonable budget and schedule.

Underpinning each of these challenges is a strategic imperative: the need to proactively aggregate knowledge as early as possible in the development process to identify and address critical issues. These issues may arise due to technical challenges, which typically receive substantial focus, or as a result of logistic, economic and financial issues, which are sometimes overlooked. It is important to develop all of these areas in parallel to generate adequate details to assess project viability.

Knowledge Transfer Process

GOAL
Facilitate the application of experience and lessons learned from engineering, procurement, construction and operations to confirm the appropriate design basis that achieves the project premise.

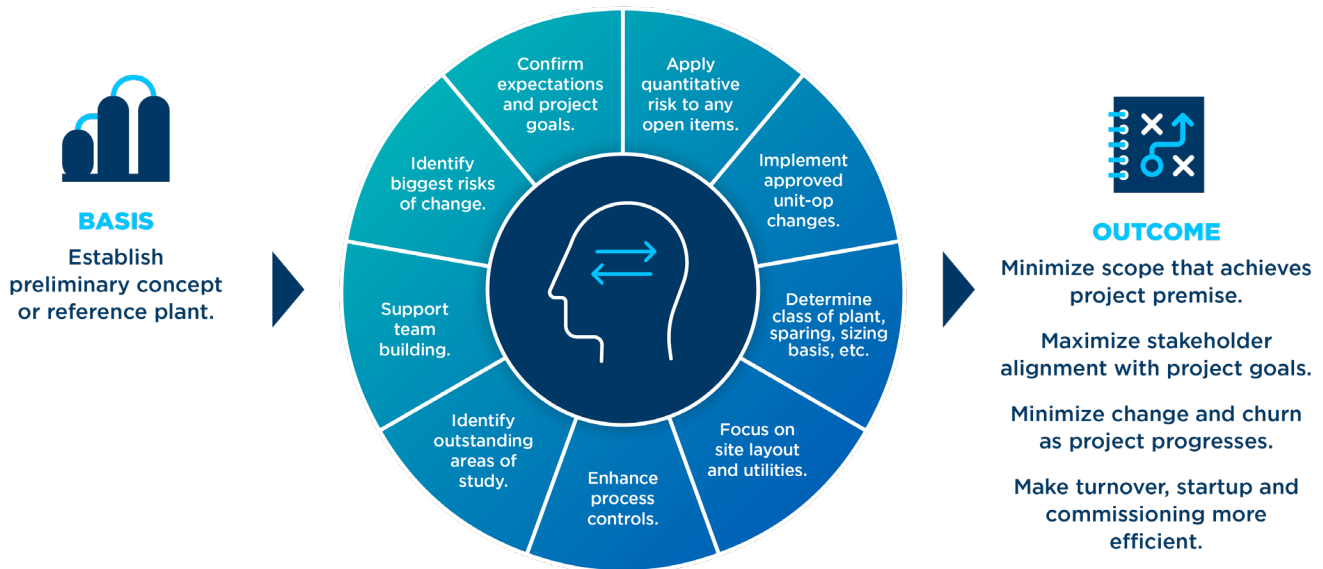


Figure 1: Knowledge transfer process.

Structured Knowledge Transfer as a Foundation for Development

First-of-a-kind projects introduce the difficulty of aggregating limited existing knowledge that may be dispersed across stakeholders, including process owners, technology vendors/licensors, the engineering team and even sister industries. As project teams encounter unfamiliar territory, information gaps and shifting priorities can lead to overlooked risks, unexpected delays and scope creep.

In this context, a structured knowledge transfer (KT) process (see Figure 1) can help bridge these gaps by systematically aggregating relevant information and highlighting areas of uncertainty. In short, this is a formal approach for identifying and prioritizing areas of technical uncertainty early in the project. A well-executed knowledge transfer session should reduce indecision, see that all parties are aligned on the project scope and save time by reducing the likelihood of rework later in the project.

For novel technologies, evidence from pilot projects is an important pillar for pinpointing critical unknown variables as early as possible. The resultant knowledge base is the foundation for an effective early-stage risk assessment.

Systematic Risk Assessment

An effective project risk analysis should center on a clearly defined process for:

- Tracking and understanding the status of process development.
- Listing issues and results to date.
- Defining and rating specific technical risks.
- Developing potential alternatives and mitigation strategies.

A gated process with well-defined evaluation points can be pivotal in deciding whether the project should move forward. This process helps generate a road map for defining the uncertainties inherent to scaling up new technologies or implementing novel processes.

The project risk analysis should encompass the project holistically, including nontechnical issues such as feedstock availability and logistics, product demand and distribution, CAPEX/OPEX targets, government incentives, and financing structure. A new process can be technically viable, meaning it works, but fails on logistic or economic grounds, leading to no money being made. The risk analysis can help address these issues early in development to see that the program is worth the investment.

It is important to note that rigorous risk analysis should not assume that mitigation strategies are capable of balancing every risk factor. Skepticism is healthy; ending a development program due to a fatal flaw is not a failure. Indeed, recognizing this flaw as early as possible in the planning process is the best way to limit unnecessary spending and should be regarded positively in a healthy organization.

Aligning the Right Resources

Engineering experience is an important foundation for performing new technology evaluations. Ideally, the engineering team should offer:

- Diverse, hands-on project experience, including knowledge of development and scale-up, as well as full-scale project execution.
- Understanding of a wide variety of unit operations, which is key for informing equipment selection and system design while incorporating lessons learned from existing technologies.
- A technology-agnostic approach backed by cross-functional knowledge and experience to facilitate collaboration and avoid premature or misguided selection of a particular technological approach or set of unit operations.
- Strong process simulation capabilities.

Beyond these fundamental capabilities, the engineering team should understand when more specialized skills will be needed, such as computational fluid dynamics (CFD) modeling, development of phase equilibria and/or reaction thermochemistry data, and reactive chemical relief evaluation, like reaction calorimetry coupled with Design Institute for Emergency Relief Systems (DIERS) relief methodology. For example, CFD modeling can be helpful in understanding multiphase fluid flow through a chemical reactor. Reaction calorimetry may be required to support safety system design for exothermic chemical reactions.

Beyond these engineering resources, broader management knowledge helps in forecasting CAPEX/OPEX, exploring feed and product logistics, conducting market research to understand target buyers and competitive financial targets, and locating funding sources for developing new technologies.

Avoiding Internal Bias in New Technology Evaluation

A cross-functional team helps avoid internal bias toward particular technological approaches. Limited experience with alternative approaches, engineers' natural pride of ownership, and desire to successfully sell the original design concept may limit the scope of the technology evaluation process. In many cases, this bias includes a narrow focus on known technologies and unit operations within the same industry — even when other industries have a long history of solving closely related engineering challenges using other methods.

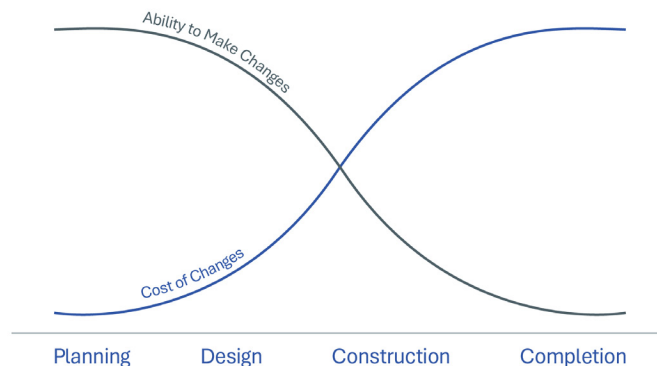


Figure 2: Cost Influence Curve.

To avoid these issues, frequent collaboration to reassess all available information and maintain a healthy skepticism is important. Novel projects demand new knowledge, and project teams must be willing to learn from relevant sister industries and borrow solutions that are already proven. If other industries have employed a similar technology or a different technology in a similar application, their hard-won knowledge should not be ignored for the sake of comfort with more familiar unit operations.

Cost Estimation

Accurate cost estimates are a key pillar for evaluating the feasibility of new processes. As such, they should be approached from several perspectives as soon as a base-case design concept is available. A comprehensive bottom-up CAPEX cost estimate should be developed for the base-case design. In parallel, a full economic model should be developed to provide an understanding of the balance required between product margin and CAPEX/OPEX costs to yield an economically viable project. The economic model can then inform the technical team with CAPEX and OPEX targets and guide decisions related to trade-offs between project scope, feedstock costs and OPEX costs. For example, it may be warranted to accept a lower product margin because the purchase of a more expensive, higher-quality feedstock allows a significant reduction in CAPEX.

CAPEX costs may easily be underestimated in the early phases due to outdated cost data and unrealistic installed-cost factors. Incomplete scope development may also lead to missed cost drivers such as:

- Ancillary process systems
- Feed/product treatment and purification
- Waste disposal
- Wastewater treatment
- Utility systems
- Logistics and storage
- Site development, including construction of roads, rail, buildings and other infrastructure

Developing a robust, holistic cost estimate as early as possible is critical due to the dynamics shown by the Cost Influence Curve, illustrated in Figure 2. Later in the development cycle, more and more costs become effectively locked in. The earlier that key parameters can be defined, the greater the opportunity for effective cost control. At a strategic level, more robust cost estimates early in the planning stage will help decision-makers better allocate limited capital.

Operational flexibility can also drive higher capital costs.

While flexible designs can help ease the implementation of future process improvements, it is also important to understand how this flexibility may drive additional costs and engineering complexity. Wherever possible, cost estimation practices should seek to quantify the incremental cost of process steps designed to provide flexibility for future improvements so that the team can assess if the cost is justified.

Common Pilot Plant Challenges

In this section, we examine the role of careful pilot plant design, data generation and testing when developing a novel process.

Common risks include pilot programs that are not run:

- Sequentially and continuously from one unit operation to the next.
- With recycles in place.
- With commercial (as opposed to research-grade) feedstocks and catalysts.
- Long enough to reach a steady state and/or observe catalyst degradation.

Additionally, if not identified and addressed, the following may yield significant, unexpected risk:

- Impurities in the commercial feed (if pilot uses a purified feedstock)
- Catalyst poisons and aging
- Side reactions
- Corrosion and fouling
- Recycle stream effects (if pilot operates without recycle streams in place)
- Safety and environmental issues

Data and Testing Development

Thorough data generation and rigorous testing protocols are essential for guiding design decisions and mitigating potential risks for development projects.

Chemical Reaction Data

Chemical reaction data is important for understanding reaction kinetics and potential side reactions. Reaction data development programs should be aware that kinetics may be masked by transport phenomena that can lead to erroneous conclusions.

Additionally, runaway reactions can be a significant safety risk for projects that include exothermic reactions. Quantifying this risk through reaction calorimetry is imperative during reactor development and basic engineering. Reactive chemical safety risks can be exacerbated if multipurpose reactors are used. Although multipurpose reactors may offer capital cost savings, they can result in higher safety risk due to more complex reaction processes.

Thermodynamic, Thermophysical and Transport Property Data

Separation and purification steps may be simplified in a pilot plant program that is primarily focused on developing reactor design data, with the result that phase equilibria and critical properties are not well understood. Separate phase equilibria measurements may be needed to provide the thermodynamic framework necessary for developing an efficient commercial-scale design for separation and purification steps.

Thermophysical and transport properties are another important factor to consider. Pilot plants are often run in a manner that yields good mass balance information, but inadequate heat balance information. Thermophysical fluid properties must be understood well enough to calculate the plant heat balance and support heat exchanger design.

A thorough testing program should systematically evaluate pilot plant data, incorporating outside laboratories as needed for testing related to phase equilibria, critical properties, reaction calorimetry, rheology and other key design data.

Facilitating Early-Stage Development

For organizations developing novel processes, incubation sites may provide a valuable foundation for supporting the next steps in the development process. For example, partnering with a tolling manufacturer may allow expansion to the next stage of scale-up for key systems and components while avoiding large capital investments in the early stages of development.

Navigating Reactor Scale Up

Stirred reactors provide an instructive example of technical issues that may emerge during the scale-up process. Experimental data for chemical reactions carried out in small bench-scale or pilot-scale reactors may be used directly for the design of full-scale reactors by making use of traditional scale-up rules. In general, a reactor scale-up involves determining the new operational times, mixing conditions and heating/cooling capacities.

Because scale-up rules are based on specific reactions with many assumptions, they should be used by experienced engineers as part of a concerted effort to review project-specific reactions and the underlying thermochemistry, kinetics, mass transfer rates, side reactions and unit operations, as well as potential misoperation and other factors.

Scale-Up Issues for Liquid and Liquid/Vapor Reactors

Mixing in liquid reactors can be governed by either mesomixing or micromixing, while liquid/vapor reactors are typically dominated by micromixing. Equal power per unit volume is often used as a scale-up criterion for chemical reactions in stirred vessels where mixing effects are important. However, the scales of turbulence and segregation are of equal importance and cannot be ignored in scale-up. Power per unit volume is only a reasonable scale-up criterion when the liquid reactor is controlled by micromixing, because in that case the mixing rate is determined by the turbulence energy dissipation rate. Mesomixing can dominate in larger reactors, affecting homogeneity and reaction rates, especially for complex reactions. In most cases, a larger stirred reactor correlates directly with worse mixing.

Temperature effects for exothermic or endothermic reactions are another important factor when scaling up reactors, as temperature uniformity may not be maintained in large reactors, particularly for highly exothermic, fast reactions. Upon scale-up of a stirred reactor, the heat transfer area of a jacketed vessel only increases by the square of the scale-up factor, whereas the reaction heat release increases by the cube of the scale-up factor. Reactor heat management is a key scale-up consideration to achieve good operability and process safety.

Scale-Up Issues for Liquid/Solid Slurry Reactors

Liquid/solid slurry reactors — unlike solid, fixed-bed catalyst reactors — share some characteristics with liquid-phase reactors. However, they often present more significant mass transfer limitations. As the solid content increases, these reactors face unique rheological concerns that can reduce reaction rates. Well-mixed conditions at scale are required to achieve the reaction rates measured in a pilot reactor.

To design energy-efficient mixing processes, quantitative information on slurry rheology and diffusion properties is essential. The particle properties — such as shape, porosity and size — play a significant role in effective diffusivity, impacting factors like porosity, tortuosity and adsorption constants.

While low-viscosity Newtonian fluids can typically be mixed with conventional systems, high-viscosity, non-Newtonian fluids often require novel mixer designs to achieve thorough homogenization. In some cases, semibatch fed reactors may be used to gradually introduce solids, reducing the time-average slurry concentration and mitigating viscosity challenges. Alternatively, rheology can be adjusted through high-shear mixing or use of extruder-type reactors to manage high solids content and maintain effective mixing.

Conclusion

While first-of-a-kind projects necessarily involve uncertainty, an organization can manage technical and economic risk using a structured knowledge transfer process, an experienced multidisciplinary team and a careful approach to technology selection. A comprehensive strategy can help limit costs, provide early identification of nonviable approaches and ultimately yield successful commercialization.

Approaching these projects with a flexible, systematic evaluation process allows engineering teams to navigate uncertainty while achieving cost-effective, scalable results in a timely manner. Whether through leveraging outside labs or drawing on lessons from sister industries, a proactive strategy for early-stage process development can transform complexity into competitive advantage, positioning organizations to unlock new opportunities in their market sector.

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