Technical & Commercial Progress in the Global Catalytic Process Industries

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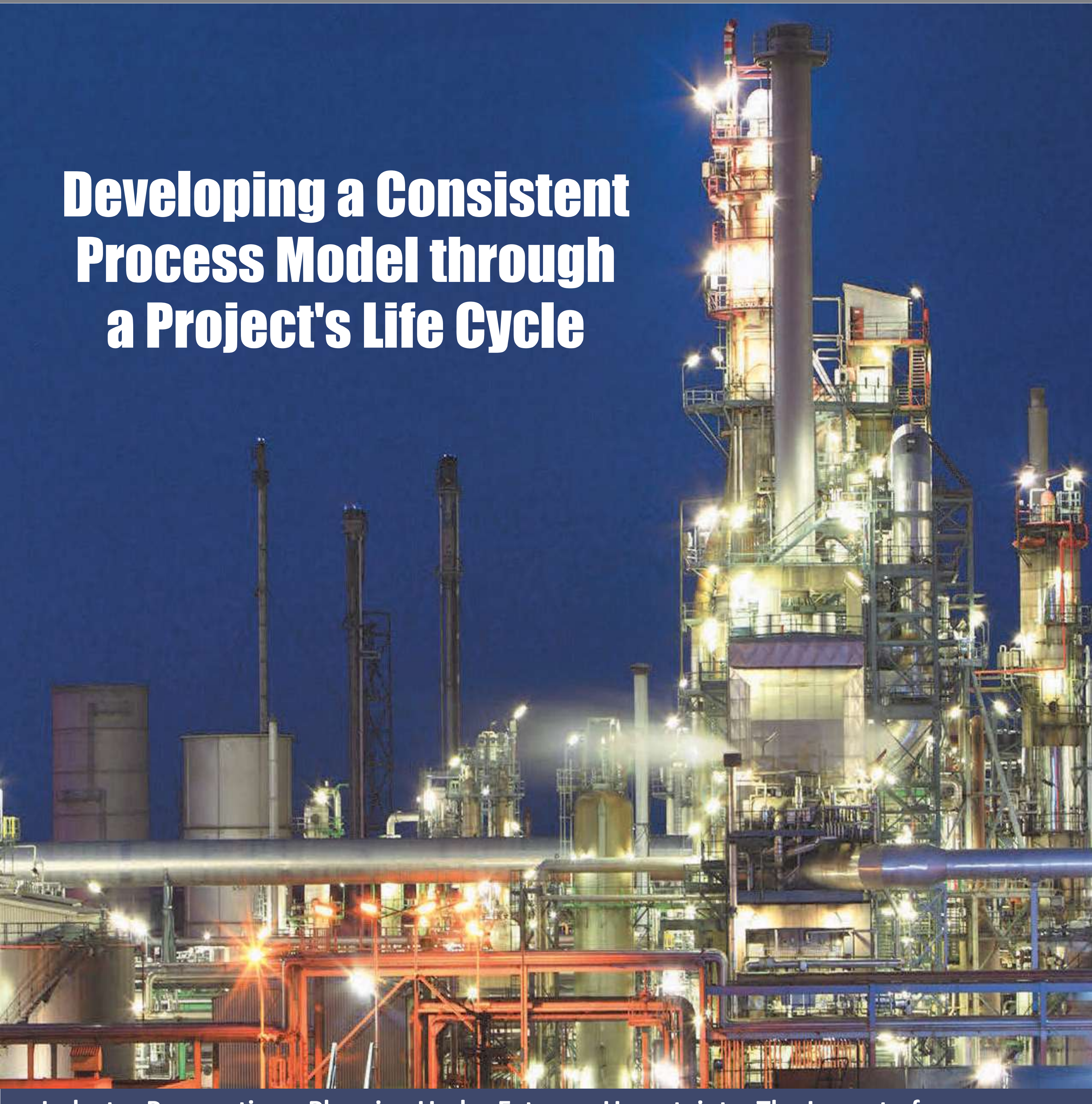
Developing a Consistent Process Model through a Project's Life Cycle



Industry Perspectives: Planning Under Extreme Uncertainty: The Impact of Low Cost and Abundant US Shale Gas and Unconventional Oil Production

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In This Issue

Developing a Consistent Process Model through a Project's Life Cycle

By Charles Sanderson

Modeling tools are deployed in both academic and industrial settings and applied to all phases of a process's development. However, the scope of value created by modeling projects is often limited to a single phase of the project or even to a specific team working on that phase. Among the reasons for this limited application are the lack of connectivity between the modeler and the broader project team, and the lack of a vision for how to leverage the model. The aim of this article is to lay out a framework to capture knowledge at each step and synthesize that knowledge into an asset, while including examples from real-world experiences.

Project Team and Phases

As a process moves through its life cycle, many disciplines are involved, each bringing different skills and perspectives. **Figure 1** illustrates how these perspectives may influence expectations. Frequently, different disciplines will favor different platforms to capture their learnings so that knowledge is dissipated as the project moves from team to team. For example, research chemists may develop reaction kinetics in a tool like MatLab but transfer only the target extent of reaction to the process design team. Process designers may develop a detailed mass and energy balance in a tool like AspenPlus, but the model is not picked up and maintained by the Operations team. The business development team may work in Excel and not take advantage of the interactions described by the engineering model. The Operations team may develop statistical models in tools like JMP but not link their insights back to fundamentals.

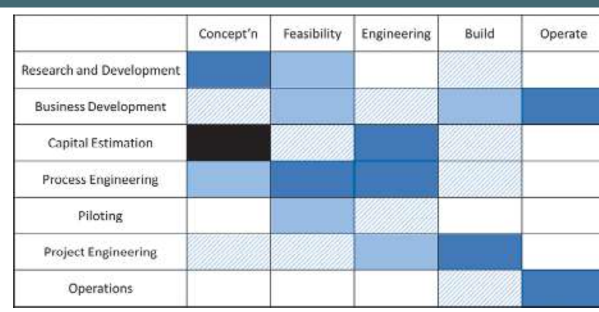
Figure 1. Different expectations that different disciplines will have from a given model; in this case a catalytic reactor.

Audience	Needs from Reactor Model
Chemist	Reaction kinetics Heat / mass transfer within catalyst Rate of catalyst degradation
Reactor Designer	Temperature / pressure / concentration profile within reactor
Process Designer	Overall conversion and heating / cooling demand from reactor Feed specification and discharge composition
Business Developer	Cost of raw materials and utilities Cost of capital Rate of production
Project Engineer	Size, pressure rating and operating temperature of equipment Piping and instrumentation requirements Ancillary equipment (e.g. pumps, valves,
Operations	Target operating point, and measurable impact of deviations Maintenance / catalyst replacement schedule

Source: Author, 2018

The focus changes as a function of maturity of the process design, and this can result in significant changes in the personnel leading and involved with the project. **Figure 2** illustrates the different phases of a typical project and the teams involved in each phase. The sections below explore a methodology that can capture much of that experience in a consistent framework, making it available throughout a process's life cycle, as simplified into the following five key steps:

Figure 2. Illustration of the phases of a project's development and the different disciplines involved in each stage. Intensity of color indicates level of involvement of different groups.



Source: Author, 2018

1. Conceptualization, where new chemistry and physics are exploited and a process flowsheet is developed to take advantage of new unit operation(s).
2. Feasibility, where the conceptual design is challenged in the real world.
3. Process Engineering, where the process design is scaled up, equipment and operating plans are developed, and capital is allocated.
4. Build and Startup, where the capital is deployed, and an operating plant is commissioned.
5. Operation, where the design exposed to real-world challenges like equipment wear, feedstock variations, changes in market conditions, and unexpected human interactions.

Process Development Requirements

Depending on the maturity of the process, the duration of, and the iteration between, steps will vary significantly. **Figure 3** illustrates some of the different activities that are involved in creating a new manufacturing plant, and illustrates how some steps may not be required for different projects:

New-to-world products, where the product is novel and a whole process must be developed. Early prototypes of the product need to be evaluated to compare them to incumbent materials. As applications are developed, preliminary quality specifications (e.g., the acceptable level of byproducts) will be set. Such projects will spend significant time in the conceptualization, feasibility, and engineering stages.

New-to-world processes, where, for example, a new catalyst that enables a new route to a product, requiring an existing process to be altered. As the modified process is developed, then new equipment may be required (e.g., pumps that can develop higher pressures or vessels that can withstand the new conditions). The project may iterate as learnings from, say, commercial feedback from possible markets requires changes in the chemistry to meet purity targets.

New technology in an existing process, where existing assets are exploited, but significant process changes are possible. For example, a new catalyst may be developed to oxidize a vent gas stream, allowing replacement of an expensive thermal oxidizer. Existing constraints, such as equipment performance, utility supply and site logistics need to be considered. Before operating at full scale, the new approach may be tested on a slip-stream. As with earlier phases, intellectual property may be developed and reduced to practice in the testing phase. Once a working demonstration has been developed, then effort will also be required to understand how to scale the equipment up to commercial capacities.

Figure 3. Activities involved in different types of process design

Source: Author, 2018

Building a new site with existing technology, where the equipment may be well understood but the design may be modified for local economics, scale, and raw materials. For an established technology, the project may start in the process engineering step, and will benefit from the already-developed process design and well-established capital estimates. The new build does offer the opportunity to incorporate learnings from the past operation of similar sites (e.g., relieving bottlenecks, incorporation of improved equipment).

Proposed Modeling Approach

Despite this difference in emphasis, a common framework and approach allows value to be created across these different projects. With the tools available today it is possible to address all these needs with a single, integrated toolset. Using a common platform facilitates knowledge transfer and minimizes transcription errors, increases the speed of a development cycle and provides all parties with a better picture of the process.

Different audiences will have different needs in terms of the appropriate level of detail. For example, the chemist may want to understand the kinetics within a reactor, while the business analyst will be satisfied with the overall yield. As such, the ideal model will allow for varying levels of detail to be incorporated into the system—equation-based tools such as Aspen Custom Modeler and gPROMS are particularly suited to this.

Conceptualization

The earliest stages of development for a new process typically involve researchers in a lab developing novel chemistry, biology or separation techniques, and business people identifying gaps in the existing markets and new applications for existing products. The goal of this phase is typically to find commercially interesting ideas for new molecules or mixtures, to create novel routes to existing chemicals, or to improve methods for separating materials.

To achieve this effectively, the team needs to develop two things: 1) A good understanding of the conditions required to achieve this novel step. This often involves physical testing in a lab, though potentially guided by computer tools such as computational fluid dynamics or hybrid approaches (e.g., high throughput screening); and 2) The economic impact of incorporating the novel step(s) into an integrated process that converts available feedstocks into marketable products.

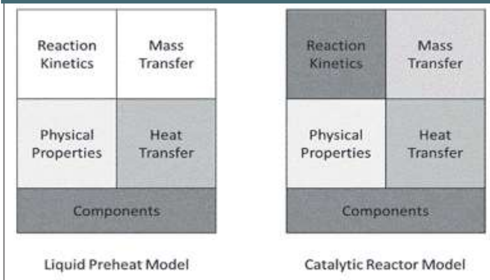
Describing the Novel Step – Unit Operation Models

During this early phase, unit operation models will be developed, and will typically incorporate (at least) five elements:

1. A set of components which generally will be distinct molecules (e.g., ethylene) but also may be composites (e.g., mixtures like “hexane” or amalgams like “catalyst”). Depending on the type of model, the components may be differentiated on some other characteristic (e.g., size of particle).
2. A set of physical properties to describe the physics of those components—enthalpy, density, viscosity, vapor pressure, and so on. Depending on the scope of the model, these properties may describe multiple phases (e.g., liquid, solid) and may describe the interaction of mixtures (e.g., the azeotrope of water and ethanol). It may be useful to “turn off” properties and regions of operation that are not required—a “catalyst,” for example, may only be physically meaningful as a solid-phase component, so there is no value in developing gas-phase correlations for it.
3. Heat transfer into and out of the modeled space and, potentially, within the unit operation (e.g., a thermal gradient within a catalyst particle).
4. Mass transfer in and out of the space, and potentially within a unit operation (e.g., mixing of two liquids in a pipe).
5. Reactions and conversion of one component to another (e.g., phase change in a crystallizer). At a minimum, reaction stoichiometry is required, but models may include reaction kinetics.

While standard unit operations (e.g., heat exchangers) may be relatively uniform across applications, more complex units (e.g., reactors) will often need to be customized for specific applications. These aspects of a unit operation model are illustrated in **Figure 4** as applied to a specific heat exchanger and catalytic reactor. For the heat exchanger, no reactions occur, and the fluids are assumed to remain well mixed, so no information on reaction kinetics or mass transfer is included. Heat transfer is described in some detail, and physical properties sufficient to describe just the liquid phase enthalpy are included. In the catalyst model, on the other hand, significant reaction detail is required as is sufficient detail to describe heat and mass transfer. In this case, the reactants are assumed not to change phase, so only a single-phase enthalpy / density description is required for physical properties.

Figure 4. Map of the aspects of a Unit Operation model. Shading indicates amount of detail included.



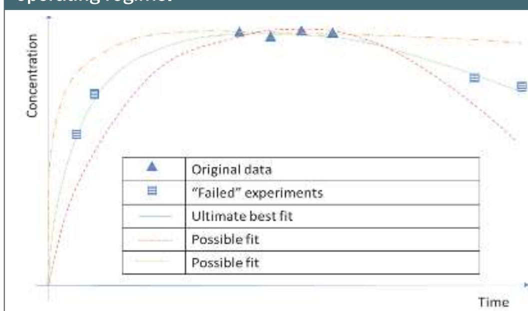
Source: Author, 2018

In the conceptualization phase, the more complex unit operations are often represented by data from batch or discontinuous operation, so it is beneficial to develop the model in a framework that can handle dynamic (time varying) as well as steady state operation. It is also sometimes necessary to develop models that include spatial variation (e.g., concentration gradients in a separation column), so an ability to solve partial differential equations is useful. Finally, there is often a need to match model predictions to experimental data, so an ability to perform data regression is attractive. AspenTech's Aspen Custom Modeler and PSE's gPROMS support all these aspects of model development, and both incorporate interfaces to physical properties databases.

Once the framework is created, the unit operation can be extended as knowledge grows. In a catalyst reaction chemistry example, one might supplement the original product-forming model with reactions forming byproducts or impurities, or one might embed the reaction kinetics into a larger model representing the catalyst packed into a reactor tube.

While developing data for the new process, one often gathers data near the expected region of operation, while experiments that fall outside this region (e.g., due to unforeseen events) are considered of limited value. A structured model, however, can often deduce much from these "failed" experiments. **Figure 5** illustrates this. If a catalyst is projected to operate near an equilibrium, for example, there's a tendency to gather data near that point. However, data from much earlier in the reaction will be far more useful in understanding the kinetics. Data gathered well after equilibrium has been reached elucidate the degradation of the products. Understanding these kinetics will in turn allow for a more powerful prediction of what will happen if the system moves to a different operating region (e.g., higher temperature, lower time). The model, therefore, can be used to help design experiments—identifying regions of experimentation that are likely to be fruitful for data regression. In the most complex cases, one may consider competing descriptions of the system (perhaps whether a reaction is following Monod or first order kinetics). Experiments can be designed using the model to maximize the difference between competing predictions.

Figure 5. Illustration of different possible fits to an original data set for a reaction product as a function of time, illustrating the benefits of data well away from the typical operating regime.



Source: Author, 2018

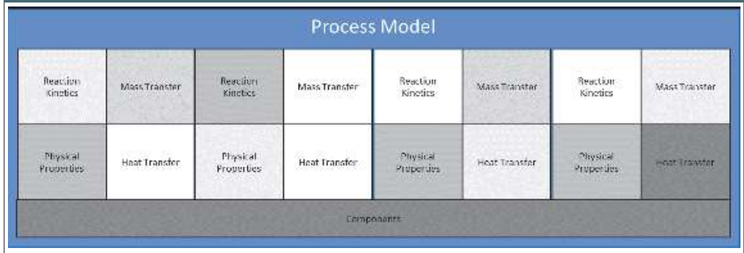
Process Development – Incorporating the Novel Step into a Design

While much of the conceptualization phase of a project will be involved with developing and understanding the chemistry and physics of the new step(s), it is important to incorporate the commercial and engineering aspects of the system as early as possible. There is a natural tendency for a team to focus on improving the performance against easily measured metrics (e.g., membrane flux) and well-defined problems (e.g., byproduct minimization), and this can lead the team to over-invest in the novel step(s) without considering the overall process. In our examples, the membrane flux may already be high enough to meet the economic targets, but the low purity may require a secondary clean-up step; or the overall amount of byproducts formed in the reactor may be reduced, but the concentration of a particularly challenging impurity may be increased. Developing an integrated process model, and overlaying process economics, early in a research project, is therefore important.

The integrated process model **(Figure 6)** may describe upstream and downstream unit operations, close recycle loops, and incorporate a description of utility demands and waste streams. Closing the overall balances can identify unexpected limitations—an impurity building up in a recycle loop, for example, or a low pH waste water stream requiring mitigation before going to a common treatment facility. It can also lead to serendipitous findings like an easily recovered coproduct or a heat recovery opportunity.

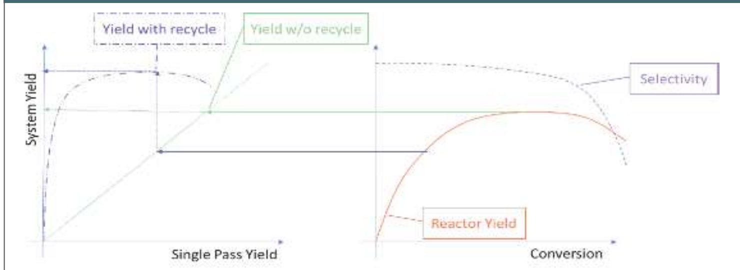
The integrated process model can therefore shift research focus and inform new process-wide metrics that address new challenges. **Figure 7** illustrates an example of reactor optimization that may occur with a catalyst driving a reaction of the form A → B → C, where B is the product of interest. In the right-hand panel, one can see that initially as A is consumed then B is formed so the yield increases. Since the concentration of B is still quite low, the rate of formation of C is also low and the selectivity (mass B / mass A consumed) remains close to 100%. As conversion increases, the concentration of B increases until C is formed more quickly than B, at which point the yield starts to drop. As the concentration of B increases, so the selectivity starts to drop, and decreases rapidly as the concentration of B increases. If one were to consider the reactor in isolation, then one would target the point of highest yield —the peak on the right-hand graph's orange, continuous line. This translates to the left-hand graph on the green curve and offers a decent yield. However, if one can identify a downstream separation step that effectively recovers unreacted A from the product mixture, then that material can be recycled for a second pass through the reactor, making more product. In this scenario, a higher overall yield can be achieved by stopping the reaction earlier, at a point of lower yield but higher selectivity, and recycling the raw material to achieve a significantly higher overall yield. The benefits of the higher yield (which will approach the selectivity for a recycle with perfect recovery) may be offset by increased reactor size or preheating, but this is nonetheless an interesting area for potential further investigation.

Figure 6. Map of an integrated process model incorporating several unit operations.



Source: Author, 2018

Figure 7. Illustration of the impact of a recycle on the overall yield in a catalytic reaction system where a raw material forms the product of interest, which then degrades to an unwanted byproduct. Stopping the reaction early, while selectivity remains high, may allow one to separate the product from the raw material, recycling the latter for a second pass through the reactor at high selectivity.



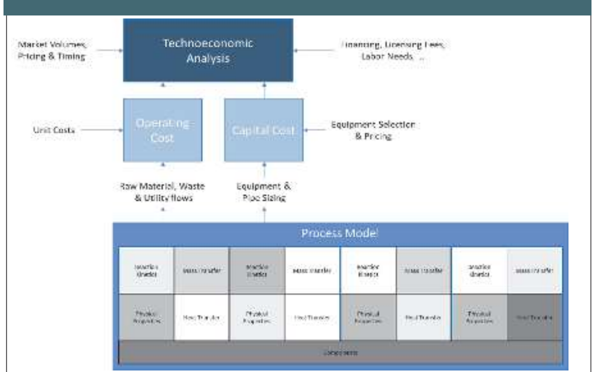
Source: Author, 2018

The integrated model can explore aspects of safety and environmental impact. For example, a solvent that works well at lab scale for dissolving a feedstock or cleaning the catalyst bed may be switched out for one that has lower toxicity or is more easily recovered. The potential for thermal runaway in a catalyst bed can be identified, and mitigation measures explored. The need for and cost of air emission handling (such as refrigerated condensation or thermal oxidizers) or waste water impurities may impact design selection.

Techno-Economic Analysis (TEA) – Overlaying the Economic Details

An integrated process model gives the team many of the key data required to develop a detailed capital and operating cost model. While such a model may only be approximate in the conceptualization phase, it can provide useful insights that can be refined in later phases of the project. The integrated model can also help to quantify other process metrics—Carbon Footprint, Life Cycle Analysis, Water Intensity, or Corporate Inventory of Target Compounds (e.g., VOCs). To address these optimizations, it makes sense to link the process model to the techno-economic analysis platform. Doing so effectively will often require detailed interaction with specialists from other fields (e.g., capital estimation or business development), so developing a handshaking tool between the process model and a more widely understood modeling environment (such as Excel), can prove useful. Ideally, this platform should be capable of being used independently from the process model but maintain its ability to be re-linked and updated as the project continues.

Figure 8. Framework linking the process model with operating and capital cost estimation to provide a techno-economic model.



Source: Author, 2018

In the spreadsheet, data from the process model (e.g., consumption rate of raw materials) can be combined with cost data (e.g., price of fuel). This can give a detailed breakdown of the variable costs for the process, and thus the production cost (e.g., $/lb product) or the projected spend rate (e.g., MM€/year). One can also pass size data into capital estimating tools, thus generating capital cost estimates, which in turn can provide inputs to the operating cost estimate (e.g., plant maintenance, insurance, depreciation). Further, one can take these data, together with projections for product sales volume and rate of market development, to develop cash flow estimates and project economic indicators such as Net Present Value or Internal Rate of Return. This part of the modeling framework is illustrated in **Figure 8.**

As with other considerations, the economic predictions can drive the core research for the process. One particularly powerful technique in this regard is Monte Carlo analysis, where the process and economic model is run many times, with key inputs being varied within given distributions. These may include process parameters (e.g., expected yield), economic parameters (e.g., market growth rate), and project parameters (e.g., time to complete piloting). The output of such an analysis is a distribution of the likely outcomes for the predictions and input factors that have the greatest impact on that distribution.

Competitive Analysis

Depending on the market for the new product, it may also be worth investigating alternative routes to the target product—how well do other catalysts perform the similar reactions? In the cases where a new route is developed for an existing product, this will be a side by side comparison of the before and after cases. The tight integration of the process and tecno-economic models allows rapid comparison of different process considerations—things like scale, feedstock composition and product specifications. It also helps guide process optimization decisions like the impact increasing catalyst loading but reducing reaction time, for example. For similar plants in different geographies, there may be significant differences in raw material/utility costs, which may drive one to make different design and operating regime choices.

For processes offering a new route to an existing molecule, it may be worth developing models of the existing processes in the marketplace. This may reveal a competitor's ability to change process conditions or product mix to open a significant margin gap, thus changing the economic targets for the new approach. It may also be worth reviewing the patent and research literature to investigate other new routes that are under development and which may have a significantly different economic structure.

Process Feasibility

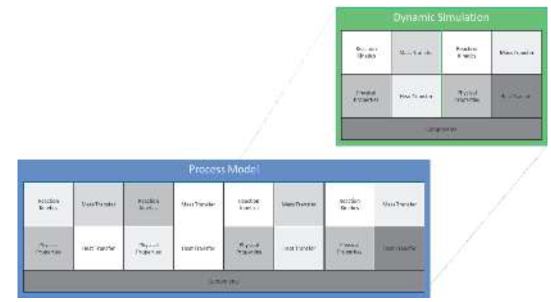
Once an economically interesting design concept is developed, it needs to be tested in the real world. This will typically take the form of a continuous benchtop system, a pilot plant, or a tolling facility. In order to make the most of such a facility, it is important to make sure that the appropriate data is gathered from the equipment and that that data is used to maximize the learnings from the piloting efforts. Again, a detailed process model, linked to a more general tool like Excel, can be a powerful tool to consolidate process and analytical data with already-existing knowledge of chemical and physical properties. Closed mass, energy and component balances may highlight important anomalies that would otherwise be missed.

At the benchtop, typically only a few steps will be integrated, and the focus of the work will be to understand process dynamics that are difficult to observe in batch systems (like impurity buildup in recycle loops), long-term operational changes (e.g., fouling of a membrane or catalyst), or phenomena difficult to isolate in simpler system (e.g., reactions during distillation). Coupling the data from such systems with a model allows the team to refine the fundamental understanding of those steps. For example, the reaction kinetic parameters that were developed in a batch system may be supplemented with equations to describe the coking of the catalyst. This in turn may drive the experimenters to identify approaches to mitigating the coking. Where recycles are closed (e.g., around a reactor, within a liquid-liquid extraction loop), impurities may concentrate to levels that allow analytical discrimination. Coupling the pilot data with the model allows one to infer the amounts of those impurities delivered with the feedstock or created in the reaction; and it allows one to regress the behavior of that impurity in the system (e.g., the vapor-liquid equilibrium).

If one is testing a new process step at an existing facility, then the process model may prove useful in planning the production campaign. Tolling equipment is rarely configured and sized in the ideal way for a new process, and the model can identify bottlenecks and other operational constraints associated with that existing equipment. Once the run is underway, the model can compare the actual results with the expected performance—for example, there may be a daily review meeting where the model framework can be used to consolidate the analytical and process data and compare the results with model predictions. This can prove useful in spotting equipment wear (e.g., a valve at an unexpected position), instrumentation drift (e.g., a weigh cell reading high), performance drift (e.g., sudden poisoning of a catalyst), or operator misunderstandings (e.g., not following an operating procedure). If a custom piloting or demonstration facility is required, then a small engineering project will be required. Since the purpose of the pilot plant will typically be to operate over a wider range of conditions than an operating facility, the model may be particularly useful in helping to adapt the design to support this flexibility. For example, additional instrumentation may be added to allow mass balances to be rigorously closed. It may also be helpful in identifying the best places within the system to perform materials testing—the section of a distillation column where an acidic component may concentrate, for example, or the part of the reactor likely to see the highest temperature. It will also enable longer term equipment testing, such as the gradual degradation of a catalyst's activity or the attrition of particles in a fluidized bed.

Most of the applications discussed for feasibility have been for steady state (time invariant) process models, but a good modeling platform allows one to convert the process description into a dynamic representation of the process. This can be particularly useful for systems that incorporate batch steps (e.g., some reactions, periodic equipment like ion exchange columns, clean-in-place cycles), or which are likely to be run as a series of campaigns designed to test the process at multiple "steady state" operating conditions (particularly common during feasibility). A dynamic simulation allows design for upstream/downstream surge capacity and development of operating procedures and schedules. While it is possible to convert the whole process flowsheet into a dynamic simulation, it's usually more expedient to use just part of the larger model (**Figure 9**); the resultant simulation will run faster and is quicker to configure.

Figure 9. Sections of the larger process model can be abstracted and used for dynamic simulation.



Source: Author, 2018

During feasibility and piloting, significant quantities of material may be produced, often under a range of operating conditions and with a range of quality parameters. These "test batches" are often very useful to develop an understanding of the new product's performance in potential applications. Feedback from these trials can provide vital information for future production and quality parameters, and a robust model can be helpful both in isolating the conditions that produce good quality product and in adjusting the design/operating conditions to achieve in-spec material. While it may involve some iteration, this approach can help avoid the need for "end of pipe" solutions. It may be possible to tweak reactor conditions, for example, to minimize an impurity level and avoid the need to add a polishing column. There may be a small drop in reactor yield, but the overall process economics may come out ahead.

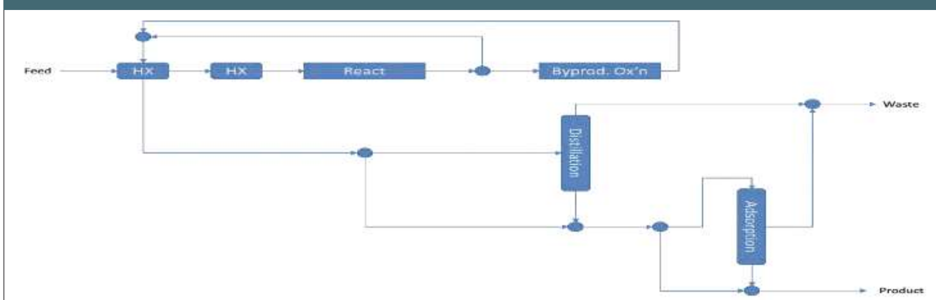
Process Engineering

Once an economically attractive process has been identified, then the work of developing a detailed engineering package for the process accelerates. This will typically have multiple phases and, for a large project, may extend over many months or years. In addition to detailed engineering deliverables (e.g., process flow diagrams, equipment data sheets), a detailed business case must be developed (e.g., cost to manufacture, capital estimates, market projections). As the engineering design develops, the core team working on the project will also evolve—less input will come from researchers and pilot engineers. As with other big shifts, this is a point where knowledge may be lost, but where a solid modeling platform can maintain a connection to key learnings.

During feasibility and the early phases of process engineering, there may be several options in play in terms of the process design, operating conditions, and equipment selection. For example, **Figure 10** shows a flowsheet with a catalytic reaction that requires a preheating step. The product has three cleanup steps that may be required in sequence or separately:

1. To pass the reactor product through a secondary reactor that oxidizes the unwanted byproduct.
2. To pass it through a distillation column to remove the byproduct
3. To pass the material through an adsorption column.

Figure 10. Simple conceptual flowsheet for a catalytic reactor and downstream cleanup system.



Source: Author, 2018

A combination of capital and operating cost estimation will help to determine where the economic optimum lies, but market development and product testing may lead to changes in product specifications while business development may impact geography and thus the raw material / utilities price and composition. In the early phases of the project engineering, a modeling platform should support switching from one design to another, allowing rapid re-evaluation of the opportunities presented within the framework of the TEA. As the design develops, the cost of making design changes increases significantly, so the more iterations that can be performed early in the design phase, the better.

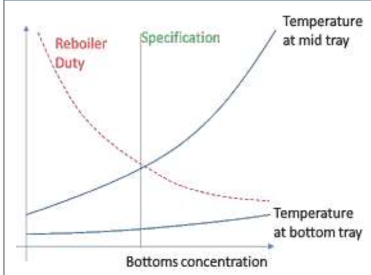
One impactful area to consider during engineering is the potential reuse and internal recycling of energy and water—in the example of **Figure 10**, the designer may choose to invest capital in a pre-heating exchanger to recover heat from the reactor discharge, thus reducing operating costs. While there are well established tools (e.g., pinch analysis), to look at heat integration, investigation early in the process design allows additional opportunities to be identified. For example, it may be possible to operate a distillation column or evaporator at a slightly higher pressure and so recover the heat into the process; or it may be possible to reuse water from a filter wash to slurry up a preceding reactor feed.

With a model that supports dynamics, the process designers can review sizing for equipment around discontinuous steps—the surge tanks isolating a dead-end filter, for example. One can also consider issues like startup, shutdown, and surge conditions. It can also be instructive to use dynamic models to investigate the performance of a process at conditions that may be experienced during market development—operating the process at turndown conditions, for example, or in campaign mode with periods of downtime.

At the more complex end, it can be valuable to leverage the model to create an Operator Training Simulation (OTS)—a dynamic representation of the process that allows users to learn from a virtual process. Such a tool can be very valuable for process engineers and operators to develop an understanding of the new process—especially powerful in new-to-the-world processes or in plants where an innovative step may have significantly changed process dynamics and responses.

Even with a steady state model, some valuable control insights can be developed. Abstractions from the detailed model may allow inferential measurements to be made (e.g., estimate the temperature inside a reactor). Correlations from the model may also be useful in equipment design, for example, density and viscosity estimates can be essential for design of mixing equipment and pumps. In more complex systems, the model can also be helpful in determining where best to put instruments—consider a distillation column designed to recover a volatile solvent from water, as in **Figure 11.** The goal is to minimize the concentration of solvent in the bottoms stream, but the bottoms temperature is relatively insensitive to the solvent level once it is below, say 99.9% —overshooting the target temperature by even a small amount (0.5°C) can greatly increase the reboiler load. Thus, a control scheme might be developed that tracks the temperature a few trays up the column, where the solvent concentration is expected to have a more significant impact on the boiling point of the mixture. With this understanding, one can develop a more responsive control scheme at the cost of a single, well-place thermocouple.

Figure 11. Illustration of using a model to identify a more sensitive control variable for a distillation column.



Source: Author, 2018

Physical property correlations, reaction kinetics and expected process conditions from the integrated process model can also provide important inputs into detailed equipment design tools that may include heat exchanger design, Computational Fluid Dynamics (CFD), and Finite Element Analysis (FEA). One might use CFD, for example, to understand the impact of geometry and impellor design on a tank then overlay reaction kinetics into that model to understand the performance of a stirred tank reactor. With the learnings from that CFD model, one can adjust the expected performance of the reactor in the process model and thus the overall process economics. As mentioned earlier, the model can support process safety and environmental considerations. It will provide estimates of gas-borne emissions (e.g., dust in a dryer exhaust), liquid discharges (e.g., consolidated waste water) and solid wastes (e.g., ash from a combustion system), and may help direct design choices. Dynamic simulation may also be useful in identifying exceptional circumstances—pH swings in discharge water during cleaning cycles, for example. From a safety perspective, the model can be a useful adjunct during process safety reviews, giving insights into the impact of unexpected conditions and even the dynamics of process failures.

Plant Operation

Once the plant starts to operate, equipment will wear, surfaces will foul, and catalysts will start to degrade. Coupling the model to plant data allows the operator to:

1. Compare current plant performance to the model predictions at those conditions, allowing the user to identify possible deviations. For example, the operator may be able to catch unexpected catalyst degradation.

Compare current plant performance to model predictions at “optimal” conditions, allowing the user to identify tweaks to process conditions that will improve performance.

2. Use the model to “look ahead” and see where the process is likely to go if no actions or if specific actions are taken.

As process economics change and different equipment becomes available, opportunities will arise to debottleneck production, to reduce energy consumption and to improve process yield. Using the model to help understand the impact of these changes, while at the same time keeping the resource in synch with the plant.

Call to Action

A structured approach can be applied to a wide range of chemical engineering projects ranging from new-to-the-world product development to improvement of well-established operations. This framework can draw together the experience of commercial, scientific and engineering team members, and provide a bridge to link the experience of the many different players in multi-year projects. The model itself provides a valuable piece of intellectual property that can be leveraged to direct research, justify investments and provide services to the process’s end users. All the aspects of the work described here have been executed on real projects with commercially available software. In my experience, it is rare that full advantage is taken of this opportunity.