Techno-Economic **Modeling for New Technology Development**

CHRIS BURK, P.E. **BURK ENGINEERING LLC** Spreadsheet software can be used to build integrated process and economic models that provide new insights into profitability.

echno-economic modeling (TEM) connects research and development (R&D), engineering, and business. By linking process parameters to financial metrics, it can help businesses better understand the factors that affect the profitability of their technology development projects.

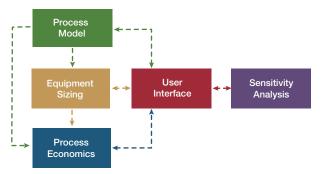
TEM is useful throughout the technology development lifecycle. When considering new ideas, innovators can use the technique to assess economic feasibility and potential. At the bench scale, scientists can use it to identify the process parameters that have the greatest effect on profitability. During process development, engineers can use TEM to compare the financial impact of different process conditions and configurations. TEM incorporates information from all of these stages of development, and offers a basis for making objective decisions.

The individual techniques used in TEM, which include process modeling, equipment sizing, and economic calculations (1-3), are already familiar to chemical engineers. This article demonstrates how to integrate and leverage them in a single, holistic model by building a techno-economic model for the fictional ABCD chemical process, which consists of four unit operations centered on a gas-phase catalytic reaction.

TEM method overview

To build a techno-economic model, you must first develop a process model and calculate equipment-sizing parameters, then estimate capital and operating costs, and finally build a user interface. The process model generates a stream table, which is the foundation of the technoeconomic model. Information from the stream table is used in equipment sizing calculations to derive parameters necessary for estimating capital and operating costs. The user interface consolidates important input and results on a single sheet, facilitating model operation and sensitivity analysis. Figure 1 shows how these components are interconnected.

Software platform. The two most common platforms for TEM are spreadsheet software and process simulation software. While each has its own benefits, this article focuses on using spreadsheet software. Spreadsheet models are flexible and do not require specialized software, so they are ideal for early-stage companies and technologies. Process simulation



▲ Figure 1. Basic structure and data flow for a spreadsheet technoeconomic model.

tends to be less accessible and to require a greater degree of certainty in process parameters and configuration, so it is generally more appropriate for later-stage projects and morecomplex systems.

Model behavior. In a techno-economic model, financial metrics are connected to process and economic parameters through a network of correlations. Automating these connections makes a model more usable and efficient. Consider how tedious it would be to collect sensitivity analysis data from a model that required you to manually enter values from equipment cost curves. In most cases, by carefully choosing methods and assumptions, you can minimize or eliminate the need for that type of manual intervention.

Accuracy. Capital cost estimates are often divided into five classifications based on accuracy (1):

- order-of-magnitude estimate (accuracy $\geq \pm 30\%$)
- study estimate (accuracy $\pm 30\%$)
- preliminary estimate (accuracy ±20%)
- definitive estimate (accuracy $\pm 10\%$)
- detailed estimate (accuracy $\pm 5\%$).

For TEM, capital cost estimates should be detailed enough to respond to changes in process parameters. However, if your estimation method is too detailed, you will have difficulty automating it. Order-of-magnitude estimates are generally not detailed enough, since they do not consider individual equipment characteristics. Preliminary, definitive, and detailed estimates are typically too detailed. Study estimates are best suited for TEM, since they account for the characteristics of individual pieces of equipment, while still allowing for automated calculation.

To develop a study estimate, first estimate major equipment costs and then apply multiplying factors to estimate total capital cost. Study estimates are also called major equipment estimates or factored estimates.

Modular structure. This article presents a modular approach to TEM. Much like in computer programming, each section or module accepts input from the user or from other sections and processes it into results for use elsewhere. The individual modules are easier to understand and error check, and, once they are built, they can be reused in future models. The screenshots in this article provide examples of how to accomplish this in a spreadsheet.

Process model

Start your techno-economic model by developing a process model. The process model calculates stream properties used to estimate equipment sizes and costs, and typically consists of a process flow diagram, user input, calculations, and a stream table. Figure 2 shows a process model for the ABCD process.

Process flow diagram. The process flow diagram

illustrates the chemical process being modeled. The new technology being evaluated might be the process itself, or it might be just one component of the process. Label all major equipment, process streams, and major utilities so they can be easily referenced. Also, include an image of the process flow diagram with the model for clarity and convenient viewing.

User input. Take extra time to identify the most appropriate user input parameters, including those that are important in other parts of your organization. For example, if business managers consider capacity in terms of product rate, do not base the model on feedstock rate. Clearly label and consolidate all user input at the top of the sheet.

Stream table. Catalog the important characteristics of each process stream in a stream table. You can perform simple material balance calculations directly within the stream table, but more complex calculations should be performed in the calculations section.

Calculations. A clearly separated calculations section reduces troubleshooting time and complexity. In general, calculations should be efficient, easy for others to understand, and fast to debug. As a first step, always convert user input to a coherent system of measurement. This section could include calculations related to chemical reactions, pressure drop, electrochemistry, and density.

Equipment sizing

To estimate equipment and utility costs, you first need to perform some equipment-sizing calculations using data from the stream table. To estimate equipment costs, calculate capacity parameters appropriate for each piece of equipment. Capacity parameters are quantitative equipment characteristics that are directly related to purchased cost. Table 1 lists typical capacity parameters and utilities for several types of equipment.

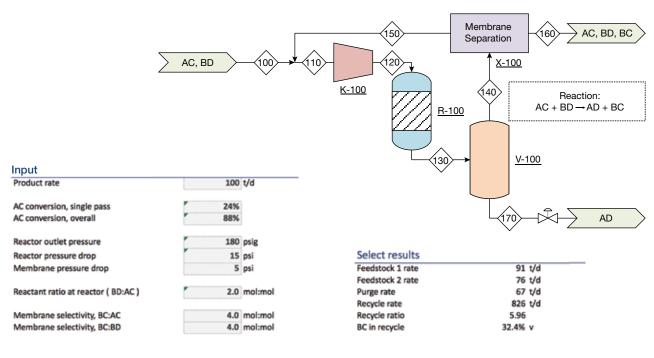
Utilities are auxiliary services, such as electricity, steam, and cooling water. To estimate utility costs, convert all utility rates to units of power (i.e., kW), then use the equation:

$$C_t = P \times C_{\varrho} \tag{1}$$

where C_t is utility cost per unit of time, P is utility rate in units of power, and C_e is utility cost per unit of energy. Values for C_e vary based on utility type and are tabulated in various sources (2).

The lack of available information in early development will require you to make some educated guesses based on experience or established heuristics. Heuristic tables (2)

Figure 3 shows the equipment sizing section of the ABCD model. Note the organization and how it provides clarity.



Stream Table

Stream			100	110	120	130	140	150	160	170
Temperature	degC		25	25	25	25	25	25	25	25
Pressure	bar		13.1	13.1	14.4	13.4	13.4	13.1	1.1	13.4
Vapor fraction			1	1	1	8.99E-01	1	1	1	0
MW	kg/kmol	•	54.3	45.9	45.9	45.9	43.8	44.5	36.7	80.0
Density	kg/m3		28.6	24.2	26.7		23.7	23.5	1.6	950.0
Mass flow rate	kg/s	•	1.93E+00 F	1.15E+01 F	1.15E+01	1.15E+01 F	1.03E+01 F	9.56E+00 F	7.70E-01 F	1.16E+00
Feedstock 1	AC		1.05E+00	3.86E+00	3.86E+00	2.93E+00	2.93E+00	2.81E+00	1.26E-01	
Feedstock 2	BD		8.76E-01	5.55E+00	5.55E+00	4.88E+00	4.88E+00	4.67E+00	2.10E-01	
Product	AD					1.16E+00				1.16E+00
Byproduct	BC			2.09E+00	2.09E+00	2.52E+00	2.52E+00	2.09E+00	4.34E-01	
Mole flow rate	kmol/s	•	3.55E-02 F	2.50E-01 F	2.50E-01	2.50E-01 F	2.36E-01 F	2.15E-01 F	2.10E-02 F	1.45E-02
Feedstock 1	AC		1.64E-02	6.03E-02	6.03E-02	4.58E-02	4.58E-02	4.38E-02	1.97E-03	
Feedstock 2	BD		1.90E-02	1.21E-01	1.21E-01	1.06E-01	1.06E-01	1.02E-01	4.57E-03	
Product	AD					1.45E-02				1.45E-02
Byproduct	BC			6.952E-02	6.952E-02	8.399E-02	8.40E-02	6.95E-02	1.45E-02	
Volume flow rate	m3/s		6.73E-02	4.75E-01	4.30E-01 F	4.37E-01	4.36E-01	4.08E-01	4.73E-01	1.22E-03

Calculations

AD density		950 kg/m3		Product rate	1.16E+00 kg/s
Reaction		Stoich. coeff.	kmol/s	AC feed to reactor	1.45E-02 kmol/s 6.03E-02 kmol/s
Feedstock 1	AC	-1	-1.45E-02	AC feed rate	1.64E-02 kmol/s
Feedstock 2	BD	-1	-1.45E-02	AC unreacted	1.97E-03 kmol/s
Product	AD	1	1.45E-02		
Byproduct	BC	1	1.45E-02	Reactor outlet pressure	1.24E+01 barg
		***************************************			1.34E+01 bar
Membrane selectivity,	BD:AC	1.00 m	ol:mol	Reactor pressure drop	1.03E+00 bar
Permeate / feed rate, /	AC	0.043		Membrane pressure drop	3.45E-01 bar
Permeate / feed rate, l	BD	0.043			
Permeate / feed rate, l	BC	0.172		Recycle ratio	5.96E+00 mass

▲ Figure 2. In the ABCD process, gaseous feedstocks AC and BD react catalytically to form liquid product AD. A membrane separation unit selectively removes byproduct BC from the recycle stream.

Capital costs

Capital costs are one-time expenses, typically incurred at the beginning of a project. They can range from thousands of dollars for small systems, to billions of dollars for a large plant. Capital costs are the investment on which economic benefits are expected to provide a return.

Total capital is the sum of fixed capital and working capital. In a study estimate, you can estimate fixed and working capital based on the summation of major equipment costs. To estimate total capital, begin by determining the major equipment costs based on the capacity parameters from the equipment sizing section.

Major equipment costs. Major equipment includes expensive pieces of equipment typically associated with unit operations, such as vessels, heat exchangers, and compressors. It does not include piping, instrumentation,

Table 1. Typical capacity parameters and utilities for various types of equipment. **Equipment Type** Capacity **Utilities Parameter** Pump, Compressor Shaft Power Electricity, Fuel Vessel, Tank, Volume Steam, Reactor Cooling Water Heat Exchanger Area Steam, Cooling Water, Refrigeration Heater Duty Electricity, Fuel Blower Standard Electricity, Fuel Volumetric Flowrate

or valves. Many correlations are available for estimating purchased equipment costs based on capacity parameters. Some are numerical and some are graphical. Numerical correlations are preferred for TEM, because you can implement them directly in a spreadsheet and they do not require user intervention. If necessary, you can plot and regress graphical correlations to give a numerical form. Figure 4 shows the major equipment cost estimation section of the ABCD model.

There are two common methods to estimate purchased equipment costs. The simpler method uses a scaling exponent to extrapolate from a baseline cost:

$$C_2 = C_1 \times (X_2/X_1)^n \tag{2}$$

where C is purchased equipment cost, X is a capacity parameter, and n is a scaling exponent. The baseline cost could come from a quote or from past cost data. The value of the scaling exponent depends on equipment type, and can vary from less than 0.3 to greater than 1. General guidelines for using this approach are widely available (1-3).

If adequate baseline cost data are not available, cost-to-capacity correlations are a good alternative (2). In addition to capacity, these correlations may also consider materials of construction, design pressure, and other factors.

Because baseline cost data and cost-to-capacity correlations typically only apply to a specific year, you need to adjust the resulting cost estimates to match current market conditions. Do this using an appropriate yearly cost index, such as the Chemical Engineering Plant Cost Index (CEPCI)

Equipment Sizing

K-100		R-100			V-100	
Offsheet references		Offsheet references			Offsheet references	
Flow rate	4.75E-01 m3/s	Flow rate	3.86E+00	kg/s	Gas flow rate	4.36E-01 m3/s
Suction pressure	1.31E+01 bar	Pressure	1.44E+01	bar	Pressure	1.34E+01 bar
Discharge pressure	1.44E+01 bar					
Input		Input			Input	
y (Cp/Cv ratio)	1.40	L/D	5.0		L/D	4.0
Shaft efficiency	65%	Fill fraction	80%		Safety factor	0.75
Drive efficiency	85%	WHSV wrt. AC	0.3	1/h	k-value	0.35 ft/s
		Catalyst density	1050	kg/m3		
		Catalyst lifetime	2.0	yr		
Calculations		Calculations			Calculations	
y/(y-1)	3.50E+00	WHSV	8.06E-05	1/s	k-value	1.07E-01 m/s
Compression ratio	1.11E+00	Catalyst charge	4.79E+04	kg	Target gas velocity	5.07E-01 m/s
			4.56E+01	m3	Transverse area	8.61E-01 m2
		Catalyst rate	2.39E+04	kg/yr		
Results		Results			Results	
Suction pressure	1.31E+06 Pa	Pressure	13.4	barg	Pressure	12.4 barg
Fluid power	914 kW	Length	12.2	m	Length	4.2 m
Shaft power	1406 kW	Diameter	2.4	m	Diameter	1.0 m
Drive power	1654 kW	Volume	57.0	m3	Volume	3.6 m3

▲ Figure 3. The ABCD process has, in essence, four pieces of major equipment, but specific sizing calculations are only necessary for the compressor (K-100), reactor (R-100), and vapor-liquid separation vessel (V-100).

or the Marshall and Swift Equipment Cost Index, and the equation:

$$C_2 = C_1 \times (I_2/I_1) \tag{3}$$

where C is the cost in year 1 or 2 and I is the cost index in year 1 or 2.

Fixed capital cost. Fixed capital includes all costs associated with purchasing equipment and construction. Although major equipment is normally the largest line item, it is typically only 20–30% of the total fixed capital cost (3).

The methods discussed in this article pertain specifically to full-scale chemical plants, but new chemical technologies do not always involve building plants. Some are improved unit operations, and others are smaller chemical-generation systems. Even if you cannot use these techniques exactly as described, they offer a starting point for improvising methods specific to your application. The most reliable cost estimates are those based on internal data from previous projects.

The simplest way to estimate fixed capital cost from major equipment cost is to use a Lang factor:

$$C_f = F_{Lang} \times \Sigma C_p \tag{4}$$

where C_f is fixed capital cost, F_{Lang} is the Lang factor, and C_p is major equipment purchased cost. The value used for

the Lang factor depends on the type of the chemical process, for example, 4.74 for a fluid processing plant, 3.63 for a solid-fluid processing plant, and 3.10 for a solid processing plant. However, the Lang factor technique does not consider any other process characteristics (2).

Figure 5 shows a more detailed approach, in which each component of the fixed capital cost is assigned an individual percentage contribution to the total fixed capital cost for the ABCD process. Reference 3 provides guidelines for using this method and percentage values for various cases.

A third and more accurate option is the module costing technique, which estimates the individual contribution of each piece of major equipment to the total fixed capital cost. Reference 2 provides guidelines and parameters for using this technique, as well as a useful spreadsheet implementation.

Working capital. Working capital refers to startup costs, and includes salaries and raw material inventories. Most of the working capital is recovered at the end of the project. For a typical chemical plant, working capital is between 15% and 20% of the fixed capital (3).

Operating costs

Operating costs can be divided into three categories: variable, fixed, and general. Variable operating costs scale with operating rate (percentage of capacity), whereas fixed operating costs do not. General operating costs are not

Equip	ment	Cost	Estim	ation

Tag		K-100	K-100d	R-100	V-100	Tag		X-100
Equipment type		Reciprocating	TEFC electric	Vert. process	Vert. process	Equipment type		Packaged membrane
		compressor	drive	vessel	vessel			separation system
Sizing parameters						Sizing parameters		
Capacity parameter		Fluid power	Shaft power	Volume	Volume	Capacity parameter		Feed rate
Capacity units		kW	kW	m3	m3	Capacity units		m3/:
Capacity		914	1,406	57.0	3.60	Capacity		0.436
Diameter	m			2.44	1.05			
Pressure	barg			13.4	12.4			
Material of construction		cs	cs	cs	cs			
Costing parameters						Costing parameters		
K1		2.2897	1.956	3.4974	3.4974	Baseline capacity		0.50
K2		1.3604	1.7142	0.4485	0.4485	Baseline cost		\$240,000
K3		-0.1027	-0.2282	0.1074	0.1074	Baseline source		ABC Engineering
						Baseline date		5/2012
Pressure factor		1.00	1.00	3.82	1.82			
Material factor		1.65	1.65	1.00	1.00	Scaling ratio		0.87
						Scaling exponent		0.50
Purchased cost						Purchased cost		
@ baseline conditions	USD 2001	\$261,429	\$123,271	\$41,317	\$6,032	@ baseline conditions		
process conditions	USD 2001	\$431,358	\$203,397	\$158,003	\$10,998	@ process conditions	USD 2012	\$224,131
	USD 2016	\$605,205	\$285,371	\$221,682	\$15,430		USD 2016	\$213,404
Documentation						Documentation		
Method: Cost-to-capacity	correlations					Method: Scaling exponer	t technique	
Reference: (2)						Reference: (3)		

▲ Figure 4. Purchased equipment costs for the compressor, reactor, and process vessel are estimated using cost-to-capacity correlations, whereas purchased cost for the membrane system is scaled from a quote.

Capital Cost Estimation

K-100	\$605,205
K-100d	\$285,371
R-100	\$221,682
V-100	\$15,430
X-100	\$213,404
otal	\$1,341,091

Component	% of total	Cost
Purchased equipment	23%	\$1,341,091
Purchased-equipment installation	8%	\$466,467
Instrumentation	9%	\$524,775
Piping	7%	\$408,158
Electrical	5%	\$291,542
Buildings	5%	\$291,542
Yard improvements	2%	\$116,617
Service facilities	14%	\$816,317
Engineering and supervision	7%	\$408,158
Construction expense	9%	\$524,775
Legal expense	2%	\$116,617
Contractor's fee	2%	\$116,617
Contingency	7%	\$408,158
Total fixed capital cost	100%	\$5,830,832

▲ Figure 5. Major purchased equipment costs for the ABCD process are the basis for estimating all other capital costs.

Operating Costs

1. Variable costs	Relative cost	USD/y
a. Raw materials	•	\$17,155,502
b. Waste treatment		\$923,284
c. Utilities		\$773,619
d. Operating labor		\$720,057
e. Direct supervisory & clerical labor	0.18 x operating labor	\$129,610
f. Maintenance & repairs	0.06 x fixed capital	\$349,850
g. Operating supplies	0.01 x fixed capital	\$52,477
h. Laboratory Charges	0.15 x operating labor	\$108,009
i. Patents and royalties	0.03 x total operating cost	\$778,792
2. Fixed costs		\$20,991,201
2. Fixed costs		\$20,334,204
a. Depreciation	-	
a. Depreciation b. Local taxes & insurance	- 0.03 x fixed capital	\$174,925
a. Depreciation b. Local taxes & insurance c. Plant overhead costs	0.03 x fixed capital 0.60 x (Line 1d + 1e + 1f)	\$174,925 \$719,710
a. Depreciation b. Local taxes & insurance	The state of the s	\$174,925 \$719,710 \$894,635
a. Depreciation b. Local taxes & insurance c. Plant overhead costs Total Fixed costs	The state of the s	\$174,925 \$719,710
a. Depreciation b. Local taxes & insurance c. Plant overhead costs Total Fixed costs 3. General costs	0.60 x (Line 1d + 1e + 1f)	\$174,925 \$719,710 \$894,635
a. Depreciation b. Local taxes & insurance c. Plant overhead costs Total Fixed costs 3. General costs a. Administrative costs	0.60 x (Line 1d + 1e + 1f) 0.15 x (Line 1d + 1e + 1f)	\$174,925 \$719,710 \$894,635 \$179,928 \$2,595,972
a. Depreciation b. Local taxes & insurance c. Plant overhead costs Total Fixed costs 3. General costs a. Administrative costs b. Distribution & marketing costs	0.60 x (Line 1d + 1e + 1f) 0.15 x (Line 1d + 1e + 1f) 0.10 x total operating cost	\$174,925 \$719,710 \$894,635 \$179,928

▲ Figure 6. The four major variable operating costs are raw materials, waste treatment, utilities, and operating labor. Operating costs also take into account fixed and general costs.

directly related to operation, but still need to be considered for a complete economic analysis.

Variable operating costs. The four major variable operating costs are raw materials, waste treatment, utilities, and operating labor. Start by estimating these based on the stream table and equipment sizing. Prices for bulk raw materials can be found in a variety of sources, both in print and on the web (4). Some of these sources provide guide-

lines for making preliminary utility and waste treatment cost estimates (2, 3).

For larger processes, you should estimate operating labor costs based on the number and character of the process steps (2, 3). According to a correlation in Ref. 2, a process comprising ten pieces of non-particulate processing equipment is estimated to require approximately three operators per shift. A process comprising eight pieces of

Capital			F	inancial par	rameters			Profitability	metrics					
Fixed		MM USD		Project lif	etme	10		NPV			MM USD			
Working		MM USD		Tax rate		45%		IRR		31.0%				
Salvage value	0.29	MM USD		Discount	rate	10%		PBP		4.38 y				
Operating costs & rev	enue							ROI		33.9%				
Variable operating		MM USD/v												
Fixed operating		MM USD/y												
Revenue		MM USD/y												
End of year		0	1	2	3	4	5	6	7	8	9	10	11	12
Operating rate				_	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Capital costs														
Fixed capital	% of total	096	60%	40%										
	MM USD		(3.50)	(2.33)	. '	- '	. '				. '			-
Working capital	% of total	25%		75%										
	MM USD	(0.29)	-	(0.87)	- '	. ,	. '	. '	. '	. ,	- '		-	1.17
Total	MM USD	(0.29)	(3.50)	(3.21)	-	-	-	-	-	-	-	-	-	1.17
Depreciation														
Schedule	% of FCI				20.0%	32.0%	19.2%	11.5%	11.5%	5.8%				
Amount	MM USD		. ,	-	1.17	1.87	1.12	0.67	0.67	0.34	- '		- '	
Operating costs														
Variable	MM USD/y	, , ,	. ,		20.99	20.99	20.99	20.99	20.99	20.99	20.99	20.99	20.99	20.99
Fixed	MM USD/y			-	4.97	4.97	4.97	4.97	4.97	4.97	4.97	4.97	4.97	4.97
Total	MM USD/y			-	25.96	25.96	25.96	25.96	25.96	25.96	25.96	25.9€	25.96	25.96
Revenue														
Gross	MM USD/y	· . ·	. ,		30.11	30.11	30.11	30.11	30.11	30.11	30.11	30.11	30.11	30.40
Net	MM USD/y	-		-	2.81	3.12	2.79	2.59	2.59	2.44	2.28	2.28	2.28	2.44
Cash flow														
Cash flow Yearly	MM USD/y	(0.29)	(3.50)	(3.21)	2.81	3.12	2.79	2.59	2.59	2.44	2.28	2.28	2.28	3.61

▲ Figure 7. A cash flow analysis combines capital cost, operating cost, and revenue to quantify the overall economic value of a technology.

non-particulate processing equipment and two pieces of particulate processing equipment is estimated to require 12 operators per shift. For smaller processes, it is best to base your estimate on experience and an understanding of the individual process.

Figure 6 shows how to estimate other variable operating costs based on the four major variable operating costs and the fixed capital cost (2, 3). Note that you need to estimate total operating cost before completing line items 1i, 3b, and 3c. Do this using the equation:

Total Operating
$$Cost = D/(1-F)$$
 (5)

where D is the sum (in dollars) of lines 1a-h, 2a-c, and 3a, and F is the fractional contribution of lines 1i, 3b, and 3c to the total operating cost (i.e., in Figure 6, F = 0.03 +0.10 + 0.05).

Fixed and general operating costs. Fixed and general operating costs do not change with operating rate. Fixed operating costs include insurance, taxes, and the operation of auxiliary facilities. General operating costs include administration, marketing, and R&D. Figure 6 shows how to estimate these costs as well.

Economic value metrics

The economic benefit of a process is typically expressed either as realized revenue or reduced costs. Economic value metrics balance these economic benefits against capital and operating costs to represent the overall economic value of a technology. Ideally, this approach provides a single metric for evaluating the technology being modeled and a basis for comparing it to alternative technologies and investment opportunities.

Revenue as an economic benefit. Revenue from product sales is the economic benefit for the case of the traditional chemical plant. In other cases, revenue comes from the sale of electricity or a different type of product or service. Revenue is an important part of the financial equation and should be estimated based on the stream table and market research. Processes that generate revenue should be evaluated as investments, using standard profitability metrics such as net present value, internal rate of return, and payback period (2). To calculate these metrics, you need to estimate yearly cash flows, as shown in Figure 7. Reference 5 discusses specific considerations in using economic value metrics in plant design applications.

Other economic benefits. Not all process technologies

generate revenue directly. Economic benefit can also come in the form of reduced capital or operating costs relative to other technologies. In cases like these, you should use net present value, equivalent capitalized cost, or equivalent operating cost as economic value metrics (2).

User interface

Process and economic parameters are now linked through your model to economic value metrics. Although the model is essentially complete, user inputs and results are scattered across a half-dozen pages. To get the most out of the model, you need a user interface.

The user interface is the dashboard through which you and your colleagues will interact with the model. Consolidate the important user input and results onto a single page, using familiar units. It is best to group and organize them in a way that is clear and easy to understand. In addition to economic value metrics, capital cost, and operating cost,

important results may also include feedstock, waste, and utility stream rates. Graphics make information easier to absorb, and can be used to show distributions of capital and operating costs or important equipment sizes.

This is the page that you will display in a meeting with your colleagues. Think about the questions that they will ask and be creative. See Figure 8 for some ideas.

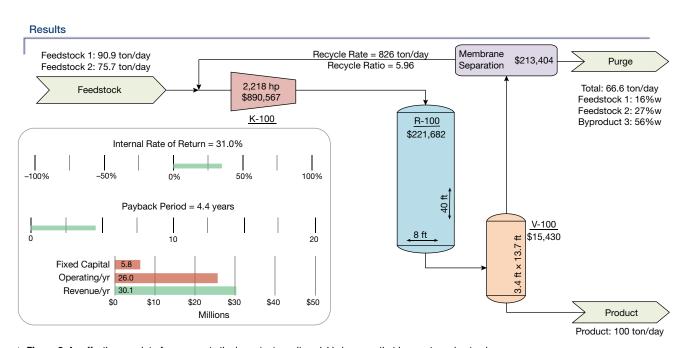
Sensitivity analysis

Sensitivity analysis investigates the impact of individual input parameters on the results of the model. It is useful for identifying opportunities and threats, as well as for understanding process dependencies. Sensitivity analysis can be performed using a tornado diagram or Excel's Data Table tool.

Tornado diagrams. A tornado diagram is a special type of bar chart that is used to compare the relative impact of input parameters on a result. The result parameter is typi-

User Interface

rocess parameters			Chemical pricing		
Feedstock 1 conversion	24%	single pass	Feedstock 1	\$425	USD/t
	88%	overall	Feedstock 2	\$110	USD/t
Reactant mole ratio	2.0	AC : BD	Catalyst	\$650	USD/t
Catalyst WHSV	0.29	1/h	Product	\$825	USD/t
Catalyst changeout period	2.0	у			
Reactor pressure	180	psig			
Reactor pressure drop	15	psi			

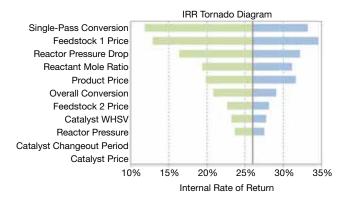


▲ Figure 8. An effective user interface presents the important results quickly in a way that is easy to understand.

cally an economic value metric. Figure 9 shows a tornado diagram for the ABCD process.

In building a tornado diagram, you specify three values for each input parameter: worst-case, expected-case, and best-case. The center axis of the tornado diagram corresponds to the expected result — the value of the result when all input parameters are set to their expected-case values. The bars extending to the left and right of the central axis reflect the relative effects of changing the input parameter to its worst-case or best-case value. Arranging the parameters in order of magnitude gives the diagram its tornado shape and highlights the most influential parameters. Reference 6 provides general instructions for building spreadsheet tornado diagrams, but certain considerations are specific to applying them in new technology development.

When interpreting a tornado diagram, consider that there are two types of input parameters: market parameters and process parameters. Market parameters include raw material and product prices and are generally outside of your control. Input case values for these parameters are set based on forecasts and historical data. A long worst-case bar next to a market parameter indicates a threat — an external factor that has a strong influence on the economic value of the process. Feedstock 1 price is an example of this in Figure 9.



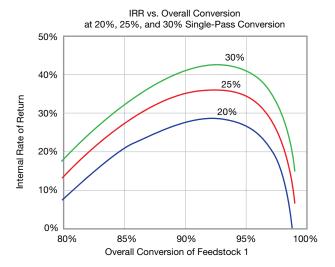
Settings	Worst	Expected	Best	Units
Single-pass conversion	15%	24%	30%	
Overall conversion	85%	88%	94%	
Reactant mole ratio	2.7	2.0	1.5	AC : CD
Catalyst WHSV	0.20	0.29	0.40	1/h
Catalyst changeout period	1.5	2.0	3.0	yr
Reactor pressure	160	180	195	psig
Reactor pressure drop	25	15	10	psi
Feedstock 1 price	\$470	\$425	\$390	USD/t
Feedstock 2 price	\$125	\$110	\$100	USD/t
Catalyst price	\$850	\$650	\$475	USD/t
Product price	\$800	\$825	\$850	USD/t

▲ Figure 9. The tornado diagram for the ABCD process highlights the relative importance of single-pass conversion and Feedstock 1 price.

Process parameters differ in that they can be changed or improved through R&D and process design. A long worst-case bar next to a process parameter indicates an opportunity and a parameter that should be targeted for improvement. Figure 9 shows this to be the case for singlepass conversion.

For process parameters, the worst case represents the current state of the technology. As progress is made toward improving a particular process parameter, the worst case will approach the expected case, and the bar representing the worst case will get shorter. The parameter will eventually drop to a lower position on the tornado diagram, indicating a decrease in relative impact.

Data tables. Excel's Data Table tool is an excellent way to perform a sensitivity analysis on one or two parameters. It automates the process of varying the input parameters and tabulating the results. Figure 10 shows a data table and graph examining the effects of overall and single-pass conversion



Data ta	ble	Sing	gle-pass convers	sion
IRR =	31%	20%	25%	30%
	80%	7%	13%	17%
	82%	14%	20%	24%
_	84%	19%	25%	30%
conversion	86%	22%	29%	35%
Ver	88%	25%	32%	38%
Ö	90%	27%	35%	41%
	92%	28%	36%	42%
Overall	94%	28%	35%	42%
٥	96%	25%	32%	39%
	98%	14%	22%	29%
	99%	-5%	6%	15%

▲ Figure 10. This data table sensitivity analysis for the ABCD process shows an optimum overall conversion between 91% and 95%, which depends slightly on single-pass conversion.

on internal rate of return for the ABCD process. Microsoft's online documentation describes the procedure for creating data tables (7).

Testing the model

Upon seeing the results of a techno-economic model for the first time, it is tempting to immediately issue a group email about the major implications you have discovered. Rest assured, though, that any reasonably complex model will initially contain mistakes and questionable assumptions. First, try to catch these yourself. The following checklist can provide a starting point.

- Process design Check with experienced engineers. Does the process flow diagram include all of the necessary equipment?
- Conceptual understanding Study different scenarios, including edge cases. Can you explain the model's behavior?
- Price Do some vendor research. Are equipment costs reasonable? Are the market data reliable?
- Historical data Look for cost data for similar processes. How do model results compare?
- Critical assumptions Use sensitivity analysis to determine the most important assumptions. How confident are you in them?

Even after thoroughly checking the model, it is wise to roll it out tentatively, with curiosity rather than deference. The results of TEM are often greeted with vigorous debate, especially if there are negative implications. At this point, it helps to have all assumptions and sources clearly documented.

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Closing thoughts

A techno-economic model embodies your best understanding of a technology, combining your knowledge of the science, the engineering, and the market. It forces you to come to terms with what you do not know, and it challenges you to either learn more or develop good assumptions.

Just as a technology evolves throughout development, so does a techno-economic model. As you learn and input new information, the model becomes more accurate. Equipment quotes lead to refined cost estimates. Lab results establish correlations between input parameters. Whether the goal is to justify an initial investment, maximize the impact of R&D efforts, or assess market readiness, TEM can help a business make better, more-informed decisions while evaluating and developing new technologies.

In a sense, the process of techno-economic modeling captures the complete engineering process, from lab to market. As a result, the developer tends to acquire a unique, holistic understanding of the technology. This perspective itself can be a great asset to any organization.

Nomenclature

C = purchased equipment cost $C_e = \text{utility cost per unit of energy}$ $C_f = \text{fixed capital cost}$ $C_p = \text{major equipment purchased cost}$ $C_t = \text{utility cost per unit of time}$ D = operating cost sum $F_{Lang} = \text{Lang factor}$ I = cost index n = scaling exponent P = utility rate in units of power Z = capacity parameter

ADDITIONAL RESOURCES

Benjamin, K. R., et al., "Use Cost Models to Guide R&D," Chemical Engineering Progress, 112 (6), pp. 44–50 (June 2016).

Clough, D. E., "Efficient Spreadsheet Use for Chemical Engineering Problem-Solving," *Chemical Engineering Progress*, **112** (8), pp. 25–34 (Aug. 2016).

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