EXAMPLE 14.1 OPTIMIZATION OF A THERMAL CRACKER VIA LINEAR PROGRAMMING

Reactor systems that can be described by a "yield matrix" are potential candidates for the application of linear programming. In these situations, each reactant is known to produce a certain distribution of products. When multiple reactants are employed, it is desirable to optimize the amounts of each reactant so that the products satisfy flow and demand constraints. Linear programming has become widely adopted in scheduling production in olefin units and catalytic crackers. In this example, we illustrate the use of linear programming to optimize the operation of a thermal cracker sketched in Figure E14.1.

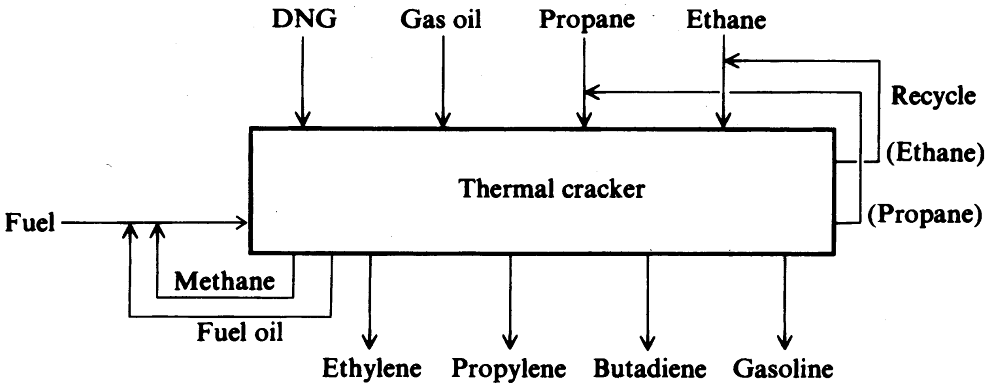

FIGURE E14.1
Flow diagram of thermal cracker.

Table E14.1A shows various feeds and the corresponding product distribution for a thermal cracker that produces olefins. The possible feeds include ethane, propane, debutanized natural gasoline (DNG), and gas oil, some of which may be fed simultaneously. Based on plant data, eight products are produced in varying proportions according to the following matrix. The capacity to run gas feeds through the cracker is 200,000 lb/stream hour (total flow based on an average mixture). Ethane uses the equivalent of 1.1 lb of capacity per pound of ethane; propane 0.9 lb; gas oil 0.9 lb/lb; and DNG 1.0.

TABLE E14.1A
Yield structure: (wt. fraction)

	Feed			
Product	**Ethane**	**Propane**	**Gas oil**	**DNG**
Methane	0.07	0.25	0.10	0.15
Ethane	0.40	0.06	0.04	0.05
Ethylene	0.50	0.35	0.20	0.25
Propane	—	0.10	0.01	0.01
Propylene	0.01	0.15	0.15	0.18
Butadiene	0.01	0.02	0.04	0.05
Gasoline	0.01	0.07	0.25	0.30
Fuel oil	—	—	0.21	0.01

Downstream processing limits exist of 50,000 lb/stream hour on the ethylene and 20,000 lb/stream hour on the propylene. The fuel requirements to run the cracking system for each feedstock type are as follows:

Feedstock type	Fuel requirement (Btu/lb)
Ethane	8364
Propane	5016
Gas oil	3900
DNG	4553

Methane and fuel oil produced by the cracker are recycled as fuel. All the ethane and propane produced is recycled as feed. Heating values are as follows:

Recycled feed	Heat produced (Btu/lb)
Natural gas	21,520
Methane	21,520
Fuel oil	18,000

Because of heat losses and the energy requirements for pyrolysis, the fixed fuel requirement is 20.0 × 10^6 Btu/stream hour. The price structure on the feeds and products and fuel costs is:

Feeds	Price (¢/lb)
Ethane	6.55
Propane	9.73
Gas oil	12.50
DNG	10.14

Products	Price (¢/lb)
Methane	5.38 (fuel value)
Ethylene	17.75
Propylene	13.79
Butadiene	26.64
Gasoline	9.93
Fuel oil	4.50 (fuel value)

Assume an energy (fuel) cost of \$2.50/10^6 Btu.

The procedure is to

1. Set up the objective function and constraints to maximize profit while operating within furnace and downstream process equipment constraints. The variables to be optimized are the amounts of the four feeds.
2. Solve using linear programming.
3. Examine the sensitivity of profits to increases in the ethylene production rate.

We define the following variables for the flow rates to and from the furnace (in lb/h):

x_1 = fresh ethane feed

x_2 = fresh propane feed

x_3 = gas oil feed
x_4 = DNG feed
x_5 = ethane recycle
x_6 = propane recycle
x_7 = fuel added

Assumptions used in formulating the objective function and constraints are

1. 20×10^6 Btu/h fixed fuel requirement (methane) to compensate for the heat loss.
2. All propane and ethane are recycled with the feed, and all methane and fuel oil are recycled as fuel.

A basis of 1 hour is used, and all costs are calculated in cents per hour.

Objective function (profit). In words, the profit f is

$$f = \text{Product value} - \text{Feed cost} - \text{Energy cost}$$

Product value. The value for each product (in cents per pound) is as follows:

Ethylene: $17.75(0.5x_1 + 0.5x_5 + 0.35x_2 + 0.35x_6 + 0.20x_3 + 0.25x_4)$ (*a*)

Propylene: $13.79(0.01x_1 + 0.01x_5 + 0.15x_2 + 0.15x_6 + 0.15x_3 + 0.18x_4)$ (*b*)

Butadiene: $26.64(0.01x_1 + 0.01x_5 + 0.02x_2 + 0.02x_6 + 0.04x_3 + 0.05x_4)$ (*c*)

Gasoline: $9.93(0.01x_1 + 0.01x_5 + 0.07x_2 + 0.07x_6 + 0.25x_3 + 0.30x_4)$ (*d*)

Total product sales $= 9.39x_1 + 9.51x_2 + 9.17x_3 + 11.23x_4 + 9.39x_5 + 9.51x_6$ (*e*)

Feed cost.

$$\text{Feed cost } (¢/\text{h}) = 6.55\text{x}_1 + 9.73\text{x}_2 + 12.50\text{x}_3 + 10.14\text{x}_4 \tag{f}$$

Energy cost. The fixed heat loss of 20×10^6 Btu/h can be expressed in terms of methane cost (5.38¢/lb) using a heating value of 21,520 Btu/lb for methane. The fixed heat loss represents a constant cost that is independent of the variables x_i, hence in optimization we can ignore this factor, but in evaluating the final costs this term must be taken into account. The value for x_7 depends on the amount of fuel oil and methane produced in the cracker (x_7 provides for any deficit in products recycled as fuel).

We combine (*e*) and (*f*) to get the objective function (¢/h)

$$f = 2.84x_1 - 0.22x_2 - 3.33x_3 + 1.09x_4 + 9.39x_5 + 9.51x_6 \tag{g}$$

Constraints.

1. Cracker capacity of 200,000 lb/h

$$1.1(x_1 + x_5) + 0.9(x_2 + x_6) + 0.9x_3 + 1.0x_4 \leq 200{,}000 \tag{h}$$

or

$$1.1x_1 + 0.9x_2 + 0.9x_3 + 1.0x_4 + 1.1x_5 + 0.9x_6 \leq 200{,}000$$

2. Ethylene processing limitation of 100,000 lb/h

$$0.5x_1 + 0.35x_2 + 0.25x_3 + 0.25x_4 + 0.5x_5 + 0.35x_6 \leq 100{,}000 \qquad (i)$$

3. Propylene processing limitation of 20,000 lb/h

$$0.01x_1 + 0.15x_2 + 0.15x_3 + 0.18x_4 + 0.01x_5 + 0.15x_6 \leq 20{,}000 \qquad (j)$$

4. Ethane recycle

$$x_5 = 0.4x_1 + 0.4x_5 + 0.06x_2 + 0.06x_6 + 0.04x_3 + 0.05x_4 \qquad (k)$$

Rearranging, (*j*) becomes

$$0.4x_1 + 0.06x_2 + 0.04x_3 + 0.05x_4 - 0.6x_5 + 0.06x_6 = 0 \qquad (l)$$

5. Propane recycle

$$x_6 = 0.1x_2 + 0.1x_6 + 0.01x_3 + 0.01x_4 \qquad (m)$$

Rearranging Equation (*m*),

$$0.1x_2 + 0.01x_3 + 0.01x_4 - 0.9x_6 = 0 \qquad (n)$$

6. Heat constraint
The total fuel heating value (THV) (in Btu/h) is given by

$$\text{THV} = \overset{\text{fuel}}{21{,}520x_7} + \overset{\text{methane from cracker}}{21{,}520(0.07x_1 + 0.25x_2 + 0.10x_3 + 0.15x_4 - 0.07x_5 + 0.25x_6)}$$

$$+ \overset{\text{fuel oil from cracker}}{18{,}000(0.21x_3 + 0.01x_4)}$$

$$= 1506.4x_1 + 5380x_2 + 5932x_3 + 3408x_4 + 1506.4x_5 + 5380x_6 + 21{,}520x_7 \qquad (o)$$

The required fuel for cracking (Btu/h) is

$$\overset{\text{ethane}}{8364(x_1 + x_5)} + \overset{\text{propane}}{5016(x_2 + x_6)} + \overset{\text{gas oil}}{3900x_3} + \overset{\text{DNG}}{4553x_4}$$

$$= 8364x_1 + 5016x_2 + 3900x_3 + 4553x_4 + 8364x_5 + 5016x_6 \qquad (p)$$

Therefore the sum of Equation (*p*) + 20,000,000 Btu/h is equal to the THV from Equation (*o*), which gives the constraint

$$-6857.6x_1 + 364x_2 + 2032x_3 - 1145x_4 - 6857.6x_5 + 364x_6$$

$$+ 21{,}520x_7 = 20{,}000{,}000 \qquad (q)$$

Table E14.1B lists the optimal solution of this problem obtained using the Excel Solven (case 1). Note that the maximum amount of ethylene is produced. As the ethylene production constraint is relaxed, the objective function value increases. Once the constraint is raised above 90,909 lb/h, the objective function remains constant.

TABLE E14.1B

Optimal flow rates for cracking furnace for different restrictions on ethylene and propylene production

	Flow rate (lb/h)	
Stream	**Case 1**	**Case 2**
x_1 (ethane feed)	60,000	21,770
x_2 (propane feed)	0	0
x_3 (gas oil feed)	0	0
x_4 (DNG feed)	0	107,600
x_5 (ethane recycle)	40,000	23,600
x_6 (propane recycle)	0	1,195
x_7 (fuel added)	32,800	21,090
Ethylene	50,000	50,000
Propylene	1,000	20,000
Butadiene	1,000	5,857
Gasoline	1,000	32,820
Methane (recycled to fuel)	7,000	19,610
Fuel oil	0	1,076
Objective function (¢/h)	369,560	298,590

Suppose the inequality constraints on ethylene and propylene production were changed to equality constraints (ethylene = 50,000; propylene = 20,000). The optimal solution for these conditions is shown as case 2 in Table E14.1B. This specification forces the use of DNG as well as ethane.

EXAMPLE 14.2 OPTIMAL DESIGN OF AN AMMONIA REACTOR

This example based on the reactor described by Murase et al. (1970) shows one way to mesh the numerical solution of the differential equations in the process model with an optimization code. The reactor, illustrated in Figure E14.2a, is based on the Haber process.

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

Figure E14.2b illustrates the suboptimal concentration and temperature profiles experienced. The temperature at which the reaction rate is a maximum decreases as the conversion increases.

Assumptions made in developing the model are

1. The rate expression is valid.
2. Longitudinal heat and mass transfer can be ignored.
3. The gas temperature in the catalytic zone is also the catalyst particle temperature.
4. The heat capacities of the reacting gas and feed gas are constant.
5. The catalytic activity is uniform along the reactor and equal to unity.
6. The pressure drop across the reactor is negligible compared with the total pressure in the system.

The notation and data to be used are listed in Table E14.2.