# **Chemical Processing Example**

In this appendix, we consider a somewhat larger problem as a medium for the discussion of the modeling process. The example is especially informative in that it incorporates a number of features found in many real-world applications.

# **Problem Statement**

A company manufactures three products X, Y and Z using raw materials A, B and C in various proportions. Products X and Y are made by a chemical process that mixes all the materials. The mixture must be at least 10% (by weight) material A and at least 5% material B. The remainder of the mixture is material C. The output of the mixture is 10% waste, 70% product X, and 20% product Y. The blending process can handle up to 10,000 pounds of input material per month.

A second chemical process that combines only materials B and C can be used to make products Y and Z. The input proportions for this process by weight are 30% material B and 70% material C. The output consists of 30% product Y and 60% product Z. The remaining 10% of the output is material A which is used in the first process.

Product X can be sold for \$5 per pound and has a maximum monthly demand of 5000 pounds. As much as 500 pounds of Y can be sold for \$11 per pound, while any additional amount can be sold for \$8 per pound. Product Z can be sold for \$10 per pound. At least 1000 pounds of product Z must be processed and sold every month.

Raw materials A, B and C can be purchased for \$4, \$3 and \$1 per pound, respectively. No more than 5000 pounds of material B can be purchased each month, while A and C are available in unlimited quantities.

The problem is to determine how much of products X, Y and Z to produce and how much of materials A, B and C to buy during the month. The objective is to maximize profit.

# Model

At first glance the analyst might list the decision variables as *X*, *Y*, *Z*, *A*, *B*, and *C* corresponding to the six problem elements, respectively. In many cases, however, clarity of modeling is served by defining extra variables not immediately apparent from the statement of the problem. The goal in modeling should be clarity rather than parsimony with respect to the number of variables and constraints. Computers are powerful enough to

allow some excesses in this regard. We often start the modeling process by defining variables for every conceivable decision. After the objective function and constraints are expressed in algebraic form, redundant or unnecessary variables can be removed.

Each variable and constraint should be assigned a name related to the quantity or restriction that it represents in the problem. It is common to use names that are abbreviations, acronyms, or a combination of letters and sequential reference numbers. General variable names such as X and Y should be avoided unless they represent, as in this problem, relevant quantities. The definition of the variables, written out in explicit terms, should accompany the model presentation.

#### Flow Diagram

When appropriate, it is useful to develop a flow diagram for the problem or process under investigation. Many scheduling, production planning, blending, network and related problems have physical input-output relationships that can be easily described with graphical constructs. A common type of input-output relationship derives from the principle of conservation of flow. The quantity being conserved can be a fluid, money, electric power, or any type of resource. A flow diagram, similar to the one shown in Fig. 19 for our problem, can be a real help in proper modeling.

As noted in Section 2.6, the circles in the figure are called nodes and the directed line segments (arrows) are called arcs. The arrangement of arcs and nodes shows the flow of materials in this problem and help to identify the variables that will be used. The model is to describe the flows at steady state so there is no logical conflict, for example, in specifying the output of node M2 as an input to node A-CON.

From the diagram we define the decision variables for the model. It is good practice to indicate the dimensional units along with the definitions. Upper case letters with no subscripts are used for variable names because this is the format required by most computer codes.

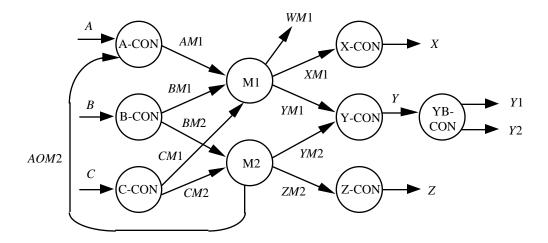


Figure 19. Flow diagram for chemical processing example

#### Variable Definitions

**Raw Materials** A, B, C : quantities of raw materials A, B and C purchased (lb.) Mixture 1 M1 : amount of mixture 1 (lb.) AM1, BM1, CM1 : quantities of raw materials A, B and C input to mixture 1 (lb.) XM1, YM1 : quantities of products X and Y produced by mixture 1 (lb.) WM1 : amount of waste produced by mixture 1 (lb.) Mixture 2 M2 : amount of mixture 2 (lb.) BM2, CM2 : quantities of raw materials B and C input to mixture 2 (lb.) YM2, ZM2 : quantities of products Y and Z produced by mixture 2 (lb.) AOM2 : quantity of raw material A produced by mixture 2 (lb.) **Finished Products** X, Y, Z: quantities of products X, Y and Z produced (lb.) *Y*1 : quantity of product Y sold for \$11 per pound (lb.) *Y*2 : quantity of product Y sold for \$8 per pound (lb.)

#### Conservation of Flow Constraints

Many of the constraints in this model are taken directly from Fig. 19. These are the conservation of material flow constraints which require that the total flow entering a node equals the total flow leaving the node. In some processes, flow may be lost due to leakage, evaporation, or spoilage, or may be increased due to synergy. Although this is not the case here, we have seen that such situations can be modeled with gain factors.

Every node in Fig. 19 generates a flow balance constraint. Each has been given a shorthand name corresponding to its purpose. In some cases, the node name and the related constraint have the same name. Every term in a constraint, including the constant on the right-hand side, must have the same dimensional units. We begin with flow balance for raw material A at node A-CON.

A-CON : 
$$A + AOM2 = AM1$$

Since solution algorithms require all variables to be presented on the lefthand side of the relational symbol with only constants on the right, we rewrite the constraint as

$$A + AOM2 - AM1 = 0. \tag{1}$$

The remainder of the conservation constraints are written in a similar manner.

B-CON: 
$$B - BM1 - BM2 = 0$$
 (2)

C-CON : 
$$C - CM1 - CM2 = 0$$
 (3)

M1-CONI: 
$$AM1 + BM1 + CM1 - M1 = 0$$
 (4)

To facilitate the presentation we have chosen to write the flow balance constraint at node M1 in two parts. Constraint (4) defines the input quantity of the first mix, hence the name M1-CONI. Together with constraint (5), conservation of flow at node M1 is assured. It is unnecessary to include an additional constraint of the form AM1 + BM1 + CM1 - WM1 - XM1 - YM1 = 0 because this is essentially what (4) and (5) say. Such a constraint would be redundant and might cause numerical difficulties for a solution algorithm.

M1-CONO: 
$$M1 - WM1 - XM1 - YM1 = 0$$
 (5)

- M2-CONI: BM2 + CM2 M2 = 0 (6)
- M2-CONO: M2 YM2 ZM2 AOM2 = 0 (7)

$$X-CON: \qquad XM1 - X = 0 \tag{8}$$

Z-CON: 
$$ZM2 - Z = 0$$
 (10)

**YB-CON**: 
$$Y - Y1 - Y2 = 0$$
 (11)

Constraint (11) equates the total *Y* with the two variables identifying the different revenues associated with the product Y.

#### Mixture Input Constraints

The next set of constraints defines the input component percentages of the two mixtures. The percentage restrictions of materials A and B in mixture 1 are given by AM1% and BM1%, respectively.

AM1%:
$$AM1$$
 $0.1M1$  or  $AM1 - 0.1M1$  $0$  $(12)$ BM1%: $BM1 - 0.05M1$  $0$  $(13)$ 

A corresponding constraint for CM1 requiring mixture 1 to be no more than 15% of material C would be redundant because the quantity of C input to mixture 1 is determined by constraint (4) in conjunction with (12) and (13).

BM2%: 
$$BM2 - 0.3M2 = 0$$
 (14)

A similar constraint for CM2 of the form CM2 - 0.7M2 = 0 would be redundant because the input quantity of material C is determined by constraint (6) in conjunction with (14).

#### Mixture Output Constraints

The following constraints define the output components of the mixtures.

$$XM1\%: XM1 - 0.7M1 = 0 (15)$$

$$YM1\%: YM1 - 0.2M1 = 0 (16)$$

Given constraints (15) and (16), the quantity of waste produced by the first process, *WM*1, is determined by constraint (5).

$$YM2\%: YM2 - 0.3M2 = 0$$
(17)

ZM2%: 
$$ZM2 - 0.6M2 = 0$$
 (18)

The value of AOM2 is determined by constraint (7) in conjunction with (17) and (18).

#### **Bound Constraints**

Lower bounds of zero on variables are handled automatically by the computational process so these constraints need not be explicitly included in a model entered into the computer. It is traditional, however, to show these constraints as part of the transcribed model. They can be stated in a general way as

Lower bounds that are greater than zero should be written out explicitly. For our problem, only the output requirement for product Z falls in this category.

ZLIM: Z 1000 (20)

Nevertheless, most software packages handle nonzero lower bounds by transforming them to zero and redefining the variables accordingly. This means that any LP can be modified so that all variables have a zero lower bound. Details are given in Chapter 4.

Similarly, most LP codes handle simple upper bounds implicitly so they do not have to be included as structural constraints. The implicit approach greatly increases the efficiency of solution algorithms. For clarity, though, we always include simple upper bounds in the transcribed model. If right-hand-side range sensitivity information is desired, these constraints should be written out explicitly since most codes only provide this type of output for structural constraints. For our problem, the bounds are as follows.

BNDM1:	<i>M</i> 1 10000	(21)
BNDY1:	<i>Y</i> 1 500	(22)
BNDX:	X 5000	(23)
BMDB:	<i>B</i> 5000	(24)

#### **Objective Function**

The final step in model formulation usually involves a statement of the objective which, for the current problem, is to maximize profit. Basic economics tells us that profit = (revenue) - (cost). In terms of the problem variables and data, we have

Maximize 
$$P = 5X + 11Y1 + 8Y2 + 10Z - 4A - 3B - 1C.$$
 (25)

Variables not shown in the objective function have zero coefficients. It is important that the higher unit revenue output for product Y, represented by Y1 with a unit revenue of 11, be sold before the lower revenue output, represented by Y2 with unit revenue of 8. Because the revenue for product Y is a concave function of sales, the linear programming solution correctly sequences the variables. If the lower revenue portion were to be sold first, the linear programming model would give erroneous results.

This completes the setup of the model. The traditional way to present the components is with the objective function first, followed by the structural constraints, the simple upper bounds, and finally the nonnegativity restrictions.

## **Modeling Considerations**

The example demonstrates that simple problem statements may give rise to surprisingly large models. This is, in fact, a very small model as linear programming goes. Practical examples can have hundreds of thousands of variables and tens of thousands of constraints. Certainly, thousands of variables and hundreds of constraints are not uncommon, and are readily solved with standard commercial software.

When one or more equality constraint appear in a model, one might wonder if some of the variables can be eliminated by substitution. If an unrestricted variable appears in an equality constraint, we can solve for that variable and then substitute it out of the model. For the case where all the variables in an equality are restricted to be nonnegative and the constraint is written (or can be rewritten) so that the right-hand side is nonnegative and all but one of the coefficients on the left have negative signs, the same approach can be taken. The variable with the positive coefficient can then be replaced in the objective function and constraints, thus eliminating one variable and one constraint.

In the chemical processing example, excluding the nonnegativity conditions and the simple bounds, 16 of the first 18 constraints are equalities and are of this form. A closer examination of those 16 constraints indicates that we could eliminate variables AM1, B, C, M1, M2, X, Y, Z and constraints (1), (2), (3), (4), (6), (8), (9), (10). Note that it is not possible, for example, to eliminate constraint (5) because once M1 is substituted out using constraint (4) we must replace it with A + AOM2 + BM1 + CM1 in (5). The resultant constraint does not satisfy the elimination criteria.

After making all possible substitutions we would be left with a total of 16 constraints as opposed to the original 24. This would reduce the size of the model considerably but, in general, it is not a good idea to do this. A great deal of mathematical manipulation is required in the process and errors are likely. In addition, it is very difficult to relate the

resulting model to the original situation. Compactness is achieved at the expense of model clarity and flexibility. If the variables have finite upper bounds, the substitution must also be made in the upper bound constraints. This will change them from simple bounds handled implicitly by the software to new, denser constraints that add to the computational burden. In such cases, the savings will be minimal.

When developing a linear programming model, the general rule is that clarity and flexibility should take priority over economy. Most practical models are created to be solved not just once, but many times with different parameter values and minor changes in the functional relationships. For instance, a production planning model may be solved each month as new demand data become available. The parameters should be easy to modify and not hidden in the mathematical structure. Moreover, variables and constraints should represent easily recognized aspects of the problem so that managers unfamiliar with linear programming can study and change the model.

The difficulty in solving a linear program depends on the number of variables and constraints, with the constraints being much more important than the number of variables. Empirical testing has shown that computation times are roughly proportional to the square of the number of constraints. Thus simple substitutions that do not compromise the clarity of the model might well be acceptable. This is especially true for restricted microcomputer codes with limited capacity.

# Solution

The solution is given in the sensitivity reports presented below. An examination of the results tells a great deal about the validity of the model. Very often an improperly stated model yields a completely illogical solution such as all zeros for the structural variables.

/ar iat	le Anal	ysis			tive Value:	136,857	
Num.	Name	Value	Status	Reduced Cost	Objective Coefficient	Range Lower Limit	Range Upper Limit
1	A	0	Lower	-3.	-4.		-1
2	В	5,000	Upper	23.	-3.	-26	- <u>122</u> 20
3	С	16,071	Basic	0.	-1.	-4	( <u>1111</u> ))
4	M1	7,143	Basic	0.	0.	-3	
5	AM1	1,548	Basic	0.	0.	-69	3
6	BM1	357	Basic	0.	0.	-57	25
7	CM1	5,238	Basic	0.	0.	-3	69
8	XM1	5,000	Basic	0.	0.	-4	
9	YM1	1,429	Basic	0.	0.	-14	
10	WM1	714	Basic	0.	0.	-29	
11	M2	15,476	Basic	0.	0.	-7	15
12	BM2	4,643	Basic	0.	0.	-23	57
13	CM2	10,833	Basic	0.	0.	-10	24
14	YM2	4,643	Basic	0.	0.	-23	57
15	ZM2	9,286	Basic	0.	0.	-12	29
16	A0M2	1,548	Basic	0.	0.	-69	171
17	X	5,000	Upper	4.07	5.	1	
18	Y	6,071	Basic	0.	0.	-19	- <u></u>
19	Z	9,286	Basic	0.	10.	-2	39
20	Y1	500	Upper	3.	11.	8	- <del></del> -2
21	Y2	5,571	Basic	0.	8.	-11	

# Constraint Analysis

		-		Shadow	Constraint	Range	Range
Num.	Name	Value	Status	Phice	Limit	Lower Limit	Upper Limit
1	A_CON	0	Equality	-1.	0.	-5,238	833
2	B_CON	0	Equality	-26.	0.	-15,714	2,500
3	C_CON	0	Equality	-1.	0.	-16,071	
4	M1_CONI	0	Equality	-1.	0.	-5,238	
5	M1_CON0	0	Equality	0.	0.		714
6	M2_CONI	0	Equality	-1.	0.	-10,833	
7	M2_CON0	0	Equality	-1.	0.	-5,238	833
8	X_CON	0	Equality	-0.93	0.	-3,793	2,000
9	Y_CON	0	Equality	-8.	0.		5,571
10	Z_CON	0	Equality	-10.	0.		8,286
11	YB_CON	0	Equality	-8.	0.		5,571
12	AM198	833	Basic	0.	0.		833
13	BM198	0	Lower	-25.	0.	-357	2,500
14	BM2%	0	Equality	-25.	0.	-15,714	2,500
15	XM198	0	Equality	0.93	0.	-2,000	625
16	YM98	0	Equality	8.	0.	-1,429	714
17	YM2%	0	Equality	7.	0.	-4,643	833
18	ZM2%	0	Equality	9.	0.	-5,238	833
19	ZLIM	9,286	Basic	0.	1,000.		9,286

Assuming that the results are not unreasonable, reviewing the solution identifies bottlenecks that hold down further improvement in the objective. In the case here, we observe that no raw material A is purchased — the required quantities are obtained as a by-product of mixture 2 — so ample quantities are still available. On the other hand, the entire supply of raw material B is used, implying that its limited availability is a bottleneck. The reduced cost for this variable indicates that profit will increase by \$23 for every extra unit of B that can obtained. If any units of A are purchased, though, the profit will decrease by \$3 per unit, slightly less than the cost of raw material A.

In general, the reduced costs reflect both the benefits of increased sales and the additional cost of the raw material. The information they provide, though, is marginal indicating how much the objective function would change with a unit change in one of the variables. For raw material B, the profit will increase linearly at a rate of \$23 up to some limit on B, but the analysis does not provide that limit. To find its value we can use trial and error and re-solve the model for different bounds, or we can explicitly include the upper bound constraint (24) B = 5000 in the model to get the necessary information. In particular, the constraint analysis would tell us the range over which the RHS value of this constraint could vary without inducing a change in the current values of the reduced costs. Having done this, we learn that the upper limit is 10,000. This means that increasing the quantify of raw material B from 5000 to 10,000 would increase the objective function by  $23 \times 5000$  or 115,000; i.e., doubling the available quantity of raw material B almost doubles the revenue. Whether this is worthwhile or even feasible depends on the cost of obtaining 5000 more units of B and the ability of the process can handle the additional volume. Recall that there is a limit of 10,000 lb. of input material per month.

The maximum production of X is also a bottleneck for the solution. The value of changing this limit is \$4.07 per unit. One might ask whether the upper bound constraint (23) is really necessary or whether it is possible to manufacture more of product X and dispose of any excess.

The constraint analysis indicates that AM1% and ZLIM are loose constraints, while BM1% is tight. The shadow prices on the conservation constraints (1) - (11) indicate the value of changing their RHS limits (currently 0). Since conservation of flow is a physical requirement, these values may not have much meaning.

When asked for the solution of a mathematical program, students will most often provide the value of the objective function at optimality. This is perhaps the least informative component of the solution. In most situations, the objective function excludes many qualitative factors important in the evaluation process but not quantifiable in terms of the variables, thus making it a poor overall measure of system performance. The second response of a student is likely to be the values of the decision variables. Although much more difficult to provide because of their number, decision variables hold important information about operating levels and raw material usage. It is essential to present these values in a format useful to a decision maker. A long list of numbers generated by a computer program provides little insight. Tables similar to those below might be constructed to summarize the results in a form that could be used by several operating departments.

Raw		From			Cost of
material	Purchases	process	Total used	Unit cost	purchases
А	0	1548	1548	\$4.00	\$0
В	5000	0	5000	3.00	15000
С	16071	0	16071	1.00	16071
Total					\$31071

Purchasing (amounts in pounds per month)

Mix 1 Production Control (amounts in pounds per month)

Mix inputs	Amount	Mix outputs	Amount
А	1548	Х	5000
В	357	Y	1429
С	5238	Ζ	0
Total	7143	Waste	714
		Total	7143

Mix 2 Production Control (amounts in pounds per month)

Mix inputs	Amount	Mix outputs	Amount
А	0	Х	0
В	4643	Y	4643
С	10833	Ζ	9286
Total	15476	RM A	1548
		Total	15476

## Sales (amounts in pounds per month)

Product	Amount	Unit	Revenue
		revenue	
Х	5000	\$5.00	\$25,000
Y basic	500	11.00	5,500
Y special	5571	8.00	44,571
Z	9286	10.00	92,857
Total			\$167,929

Management (	(\$ per month)
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Output measure	Amount
Revenue	\$167,929
Raw material cost	\$31,071
Operating margin	\$136,857

The least frequent student response, and perhaps the most important in practice, is a careful analysis of the system in terms of its limits. What decision variables are zero? Perhaps the system can be simplified by not providing so many options. What constraints are loose? Increasing the efficiencies in parts of the system that are not limiting is worthless. What variable upper bounds and what constraints are tight? This type of information illuminates perhaps the most fruitful areas for analysis because efforts to improve a system should focus on its bottlenecks not its operating levels.

- 11. Solve the chemical processing example in Section 2.8 using a computer program. Investigate the effect of the following changes separately. The changes are not cumulative.
  - a. Eliminate the upper bound on sales for product X.
  - b. Eliminate the upper bound on the manufacture of X, but assume any amount produced over 5000 must be discarded at a cost of \$1/lb.
  - c. Eliminate the restriction on the amount of raw material B that can be purchased.
  - d. Change the cost of raw material C to \$5/lb.