

OPTIMIZATION OF CHEMICAL ENGINEERING PROCESSES

INTRODUCTION:

OPTIMIZATION is the use of specific methods to determine the most cost-effective and efficient solution to a problem or design for a process. This technique is one of the major quantitative tools in industrial decision making. A wide variety of problems in the design, construction, operation, and analysis of chemical plants (as well as many other industrial processes) can be resolved by optimization. The goal of optimization is to find the values of the variables in the process that yield the best value of the performance criterion. A trade-off usually exists between capital and operating costs. The described factors-process or model and the performance criterion-constitute the optimization "problem."

Typical problems in chemical engineering process design or plant operation have many (possibly an infinite number) solutions. Optimization is concerned with selecting the best among the entire set by efficient quantitative methods.

Computers and associated software make the necessary computations feasible and cost effective. To obtain useful information using computers, however, requires;

- i. critical analysis of the process or design,
- ii. insight about the appropriate performance objectives i.e., what is to be accomplished, and
- iii. use of past experience, sometimes called engineering judgment.

WHY OPTIMIZE?

Engineers work to improve the initial design of equipment and strive to enhance the operation of that equipment once it is installed so as to realize the largest production, the greatest profit, the minimum cost, the least energy usage, and so on. Monetary value provides a convenient measure of different but otherwise incompatible objectives, but not all problems have to be considered in a monetary (cost versus revenue) framework.

In plant operations, benefits arise from improved plant performance, such as improved yields of valuable products (or reduced yields of contaminants), reduced energy consumption, higher processing rates, and longer times between shutdowns.

Optimization can also lead to reduced maintenance costs, less equipment wear, and better staff utilization. In addition, intangible benefits arise from the interactions among plant operators, engineers, and management. It is extremely helpful to systematically identify the objective, constraints, and degrees of freedom in a process or a plant, leading to such benefits as improved quality of design, faster and more

reliable troubleshooting, and faster decision making.

EXAMPLES OF APPLICATIONS OF OPTIMIZATION;

Optimization can be applied in numerous ways to chemical processes and plants, typical projects in which optimization has been used include

1. Determining the best sites for plant location.
2. Routing tankers for the distribution of crude and refined products.
3. Sizing and layout of a pipeline.
4. Designing equipment and an entire plant
5. Scheduling maintenance and equipment replacement.
6. Operating equipment, such as tubular reactors, columns, and absorbers.
7. Evaluating plant data to construct a model of a process.
8. Minimizing inventory charges.
9. Allocating resources or services among several processes.
10. Planning and scheduling construction.

These examples and many more not listed provide an introduction to the types of variables, objective functions, and constraints of optimization problem.

GENERAL PROCEDURE FOR SOLVING OPTIMIZATION PROBLEMS

No single method or algorithm of optimization can be applied efficiently to all problems. The method chosen for any particular case depends primarily on;

- i. the character of the objective function and whether it is known explicitly,
- ii. the nature of the constraints, and
- iii. the number of independent and dependent variables.

The six general steps for the analysis and solution of optimization problems are given below.

1. Analyze the process itself so that the process variables and specific characteristics of interest are defined; that is, make a list of all of the variables.
2. Determine the criterion for optimization, and specify the objective function in terms of the variables defined in step 1 together with coefficients. This step provides the performance model (sometimes called the economic model when appropriate).
3. Using mathematical expressions, develop a valid process or equipment model that relates the input-output variables of the process and associated coefficients. Include both equality and

inequality constraints. Use well-known physical principles (mass balances, energy balances), empirical relations, implicit concepts, and external restrictions. Identify the independent and dependent variables to get the number of degrees of freedom.

4. If the problem formulation is too large in scope:
 - i. break it up into manageable parts or
 - ii. simplify the objective function and model
5. Apply a suitable optimization technique to the mathematical statement of the problem.
6. Check the answers, and examine the sensitivity of the result to changes in the coefficients in the problem and the assumptions.

The cited order may not be followed exactly, but all the steps should be covered. Shortcuts in the procedure are allowable, and the easy steps can be performed first. The general objective in optimization is to choose a set of values of the variables subject to the various constraints that produce the desired optimum response for the chosen objective function.

Steps 1, 2, and 3 deal with the mathematical definition of the problem, that is, identification of variables, specification of the objective function, and statement of the constraints.

Step 4 suggests that the mathematical statement of the problem be simplified as much as possible without losing the essence of the problem.

Step 5 involves the computation of the optimum point. Here, quite a few techniques exist to obtain the optimal solution for problems such as;

- i. Optimization of Unconstrained Functions: One-Dimensional Search
- ii. Unconstrained Multivariable Optimization
- iii. Linear Programming (LP) and Applications
- iv. Nonlinear Programming with Constraints
- v. Mixed-Integer Programming
- vi. Global Optimization for Problems with Continuous and Discrete Variables

Several methods for handling the problems stated above will be examined later when considering Optimization as a course in higher undergraduate level. And among these methods are the use of computer applications, some of which will be considered here.

OPTIMIZATION WITH EXCEL SOLVER

Microsoft Excel solver is a powerful add-on tool to solve and analyze optimization problems. Optimization deals with selecting the best option among a number of possible choices that are feasible or don't violate constraints. Solver can be used to adjust parameters in a model to best fit data, increase profitability of a potential engineering design, or meet some other type of objective that can be described mathematically in a spreadsheet. In addition to solving equations, the Excel solver allows us to find solutions to optimization problems of all kinds (single or multiple variables, with or without constraints).

Product Mix Example

This part of our Solver Tutorial takes you step by step through the process of creating a Solver model, using a Product Mix example. We'll first consider how to define the problem and write out formulas for the objective and constraints.

Problem 1: Imagine that you manage a factory that produces four different types of wood paneling. Each type of paneling is made by gluing and pressing together a different mixture of pine and oak chips. The following table summarizes the required amount of gluing, pressing, and mixture of wood chips required to produce a pallet of 50 units of each type of paneling:

	Resources Required per Pallet of Paneling Type			
	Tahoe	Pacific	Savannah	Aspen
Glue (quarts)	50	50	100	50
Pressing (hours)	5	15	10	5
Pine chips (pounds)	500	400	300	200
Oak chips (pounds)	500	750	250	500

In the next production cycle, you have 5,800 quarts of glue; 730 hours of pressing capacity; 29,200 pounds of pine chips; and 60,500 pounds of oak chips available. Further assume that each pallet of Tahoe, Pacific, Savannah, and Aspen panels can be sold for profits of \$450, \$1,150, \$800, and \$400, respectively.

Solution: Before we implement this problem statement in either Excel, let's write out formulas corresponding to the verbal description above.

Let X_1 = Number of Tahoe pallets produced

X_2 = Number of Pacific pallets produced

X_3 = Number of Savannah pallets produced

X_4 = Number of Aspen pallets produced,

Therefore, the **objective function** is to: **Maximize: $450 X_1 + 1150 X_2 + 800 X_3 + 400 X_4$**

A pallet of each type of panel requires a certain amount of glue, pressing, pine chips, and oak chips. Therefore, the constraints for this problem can be expressed as follows:

Subject to:

$$50 X_1 + 50 X_2 + 100 X_3 + 50 X_4 \leq 5800 \quad (\text{Glue})$$

$$5 X_1 + 15 X_2 + 10 X_3 + 5 X_4 \leq 730 \quad (\text{Pressing})$$

$$500 X_1 + 400 X_2 + 300 X_3 + 200 X_4 \leq 29200 \quad (\text{Pine chips})$$

$$500 X_1 + 750 X_2 + 250 X_3 + 500 X_4 \leq 60500 \quad (\text{Oak chips})$$

Since the number of products built cannot be negative, we'll also have non-negativity conditions on the variables:

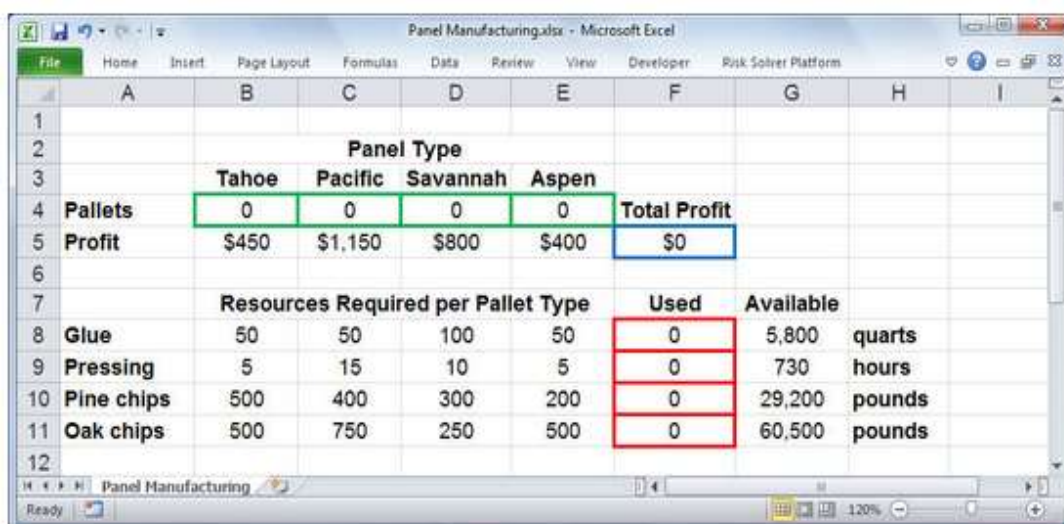
$$X_1, X_2, X_3, X_4 \geq 0.$$

Using Excel's Built-In Solver - Product Mix Example:

Essential Steps: To define an optimization model in Excel you'll follow these essential steps:

1. Organize the data for your problem in the spreadsheet in a logical manner.
2. Choose a spreadsheet cell to hold the value of each decision variable in your model.
3. Create a spreadsheet formula in a cell that calculates the objective function for your model.
4. Create a formulas in cells to calculate the left hand sides of each constraint.
5. Use the dialogs in Excel to tell the Solver about your decision variables, the objective, constraints, and desired bounds on constraints and variables.
6. Run the Solver to find the optimal solution.

Creating an Excel Worksheet:



- ❖ Cells B4, C4, D4 and E4 are to represent our decision variables X1, X2, X3, and X4 i.e representing the number of pallets of each type of panel to produce. The Solver will determine the optimal values for these cells.
- ❖ Formula for cell F5 (Total Profit): $=B5*B4+C5*C4+D5*D4+E5*E4$
- ❖ or equivalently, F5 (Total Profit): $=SUMPRODUCT(B5:E5,B4:E4)$
- ❖ Formula for cell F8: $=SUMPRODUCT(B8:E8,$B$4:$E$4)$
- ❖ The formula in F8 can now be drag for F9:F11
- ❖ In cells G8:G11, we've entered the available amount of each type of resource (corresponding to the right hand side values of the constraints).

Understanding the Excel Solver Dialogs:

- ❖ Click Solver button on the Excel Data tab, to displays the Solver Parameters dialog.
- ❖ In the Set Objective (or Set Target Cell) edit box, we type or click on cell F5, the objective function.
- ❖ In the By Changing Variable Cells edit box, we type B4:E4 or select these cells with the mouse.

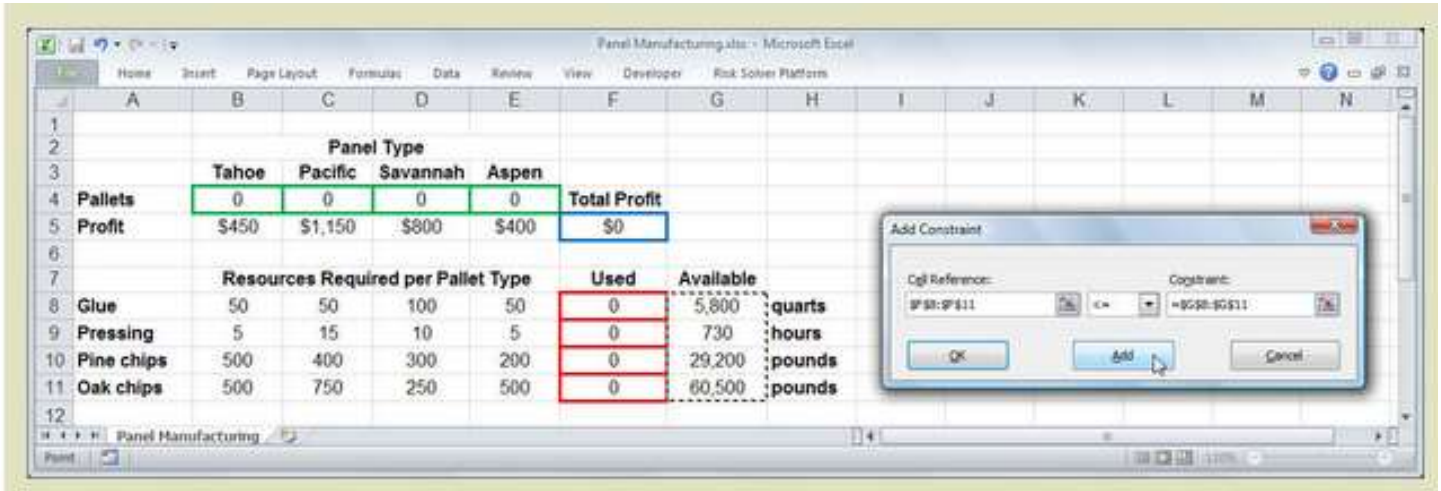
The screenshot shows the Excel Solver Parameters dialog box. The spreadsheet data is as follows:

		Panel Type					
		Tahoe	Pacific	Savannah	Aspen	Total Profit	
4	Pallets	0	0	0	0		
5	Profit	\$450	\$1,150	\$800	\$400	\$0	
		Resources Required per Pallet Type				Used	Available
8	Glue	50	50	100	50	0	5,800
9	Pressing	5	15	10	5	0	730
10	Pine chips	500	400	300	200	0	29,200
11	Oak chips	500	750	250	500	0	60,500

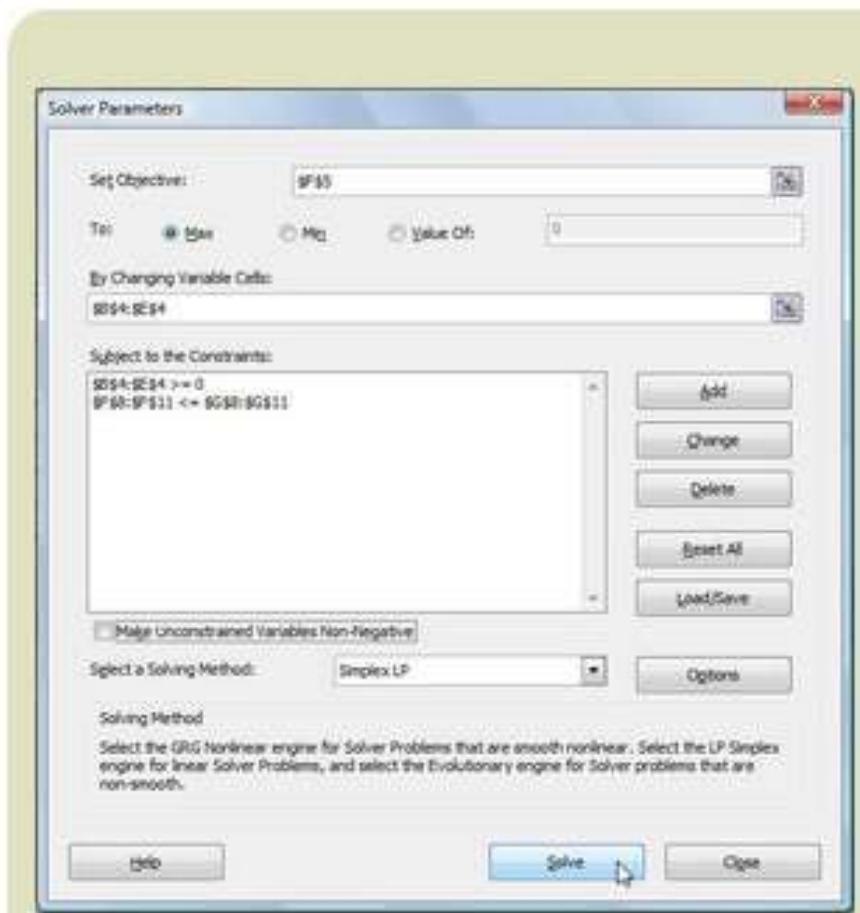
The Solver Parameters dialog box is configured with the following settings:

- Set Objective: $\$F\5
- To: Max Min Value Of:
- By Changing Variable Cells: $\$B\$4:\$E\4
- Subject to the Constraints: (Empty list)
- Make Unconstrained Variables Non-Negative
- Select a Solving Method: Simplex LP
- Solving Method: Select the GRG Nonlinear engine for Solver Problems that are smooth nonlinear. Select the LP Simplex engine for linear Solver Problems, and select the Evolutionary engine for Solver problems that are non-smooth.

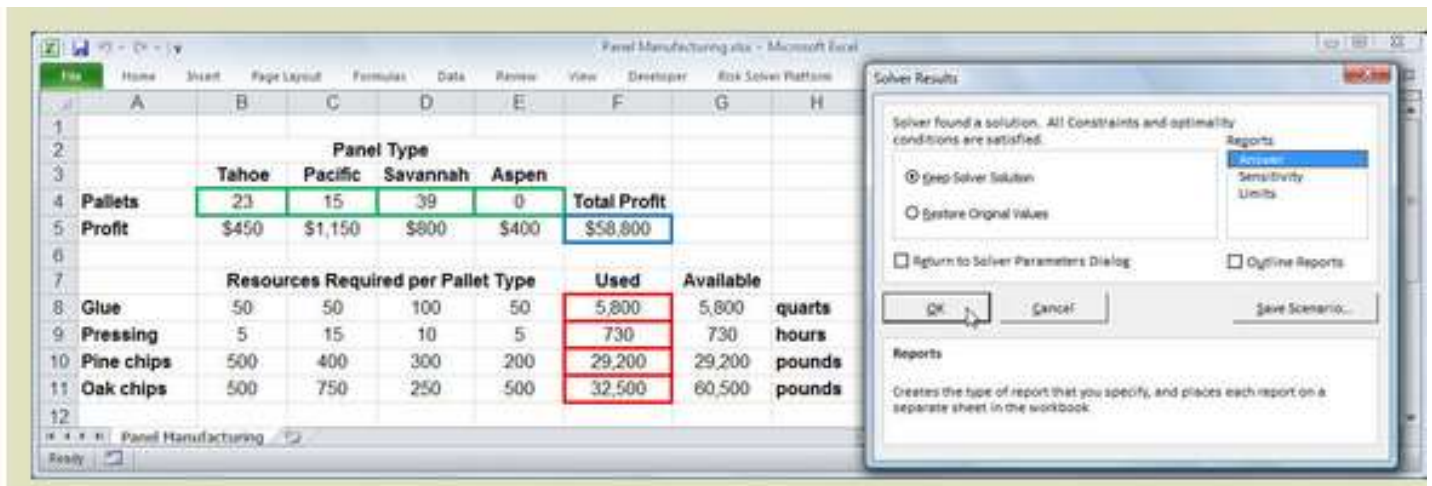
- ❖ To add the constraints, we click on the Add button in the Solver Parameters dialog and;
 - select cells F8:F11 in the Cell Reference edit box (the left hand side)
 - select cells G8:G11 in the Constraint edit box (the right hand side)
 - the default relation as \leq
 - press OK.



- ❖ We choose the Add button again (either from the Add Constraint dialog above, or from the main Solver Parameters dialog) to define the non-negativity constraint on the decision variables.

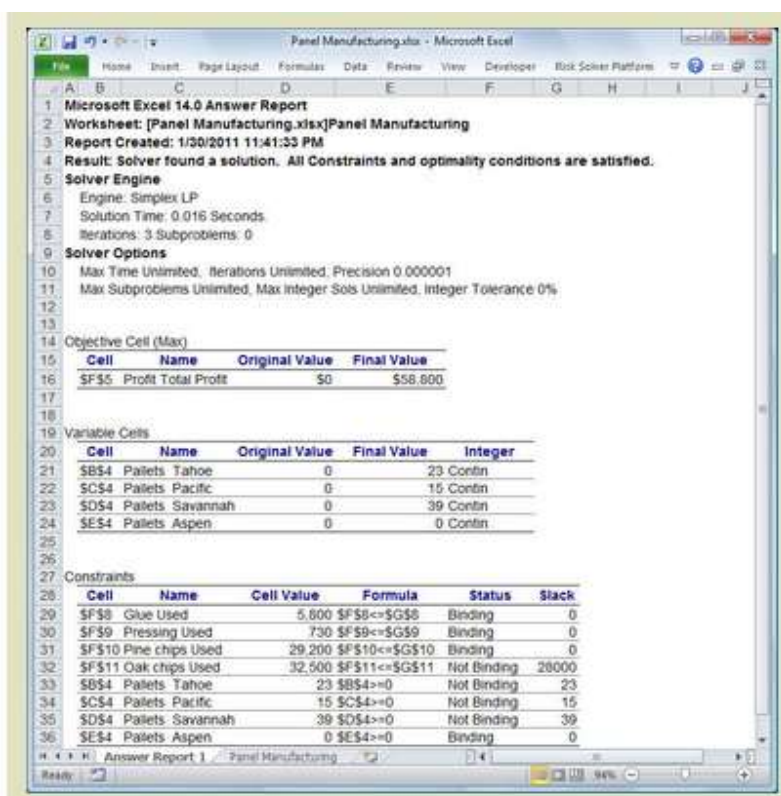


- ❖ To find the optimal solution, simply click on the Solve button. After a moment, the Excel Solver returns the optimal solution in cells B4 through E4.
- ❖ This means that we should build 23 pallets of Tahoe panels, 15 pallets of Pacific panels, 39 pallets of Savannah panels, and 0 pallets of Aspen panels. This results in a total profit of \$58,800 (shown in cell F5).



The message "Solver found a solution" appears in the Solver Results dialog, as shown above. We now click on "Answer" in the Reports list box to produce an Answer Report, and click OK to keep the optimal solution values in cells B4:E4.

After a moment, the Solver creates another worksheet containing an Answer Report, like the one below, and inserts it to the left of the problem worksheet in the Excel workbook.



Solver Parameters

Set Objective:

To: Max Min Value Of:

By Changing Variable Cells:

Subject to the Constraints:

\$B\$10 = 40
 \$B\$5:\$E\$5 <= 5
 \$B\$5:\$E\$5 >= 1
 \$B\$9 >= 25

Make Unconstrained Variables Non-Negative

Select a Solving Method:

Solving Method
 Select the GRG Nonlinear engine for Solver Problems that are smooth nonlinear. Select the LP Simplex engine for linear Solver Problems, and select the Evolutionary engine for Solver problems that are non-smooth.

Microsoft Excel 2010 ribbon: FILE, HOME, INSERT, PAGE LAYOUT, FORMULAS, DATA, REVIEW

Formulas tab: From Access, From Web, From Text, From Other Sources, Existing Connections, Refresh All, Connections, Properties, Edit Links, Sort

Formula Bar: B11

	A	B	C	D	E	F	G
1							
2							
3	Variables	X1	X2	X3	X4	Mini	
4	Lower	1	1	1	1		
5	Values	1	4.744	3.82	1.38	17.01	
6	Upper	5	5	5	5		
7							
8		Constraints					
9	1	24.9999863	>=	25			
10	2	40.0000176	=	40			

Microsoft Excel 2010 ribbon: FILE, HOME, INSERT, PAGE LAYOUT, FORMULAS, DATA, REVIEW

Formulas tab: From Access, From Web, From Text, From Other Sources, Existing Connections, Refresh All, Connections, Properties, Edit Links, Sort, Filter

Formula Bar: A60

Microsoft Excel 10.0 Answer Report

Worksheet: [CBE 302.xlsx]Sheet1

Report Created: 23-May-20 10:33:43 AM

Result: Solver found a solution. All Constraints and optimality conditions are satisfied.

Solver Engine

Engine: GRG Nonlinear
 Solution Time: 0.343 Seconds
 Iterations: 6, Subproblems: 0

Solver Options

Max Time Unlimited, Iterations Unlimited, Precision 0.000001, Use Automatic Scaling
 Convergence 0.0001, Population Size 100, Random Seed 0, Derivatives Forward, Require Bounds
 Max Subproblems Unlimited, Max Integer Sols Unlimited, Integer Tolerance 1%, Assume Nonnegative

Objective Cell (fmla):
 -Cell Name original Value
 -\$F\$5 Value Min 17.010000

Variable Cells

Cell Name	original Value	final Value	Integer
-\$B\$5 Value \$X1	1	1	1
-\$C\$5 Value \$X2	5	4.7436688	Contin
-\$D\$5 Value \$X3	5	3.8202787	Contin
-\$E\$5 Value \$X4	5	1.3795278	Contin

Constraints

Cell Name	Cell Value	Formula	Status	Blank
-\$B\$10 Constraint	40.0000176	=\$B\$10=40	Binding	0
-\$D\$5 Constraint	24.9999863	=\$D\$5>=25	Binding	0
-\$B\$5 Value \$X1	1	=\$B\$5<=5	Not Binding	4
-\$C\$5 Value \$X2	4.7436688	=\$C\$5<=5	Not Binding	0.2663314
-\$D\$5 Value \$X3	3.8202787	=\$D\$5<=5	Not Binding	1.1797213
-\$E\$5 Value \$X4	1.3795278	=\$E\$5<=5	Not Binding	3.6204724
-\$B\$5 Value \$X1	1	=\$B\$5>=1	Binding	0
-\$C\$5 Value \$X2	4.7436688	=\$C\$5>=1	Not Binding	2.7436688
-\$D\$5 Value \$X3	3.8202787	=\$D\$5>=1	Not Binding	2.8202787
-\$E\$5 Value \$X4	1.3795278	=\$E\$5>=1	Not Binding	0.3795278