ChE 32000 Optimization Project (Spring 2017)

Due Date: 11:59 p.m., April 28, 2017

Project Description

Upon logging into the following website, you will be presented with 15 factors determined to be potentially influential in the production yield for a trans-esterification plant described below. Your task is to use design of experiments (DOE) to effectively screen and optimize the factors in order to maximize your production yield.

https://engineering.purdue.edu/~che320/project/reactor

You can use JMP to set up your DOE, then, using the website, you will be able to run a single experiment at a time or schedule many experiments at once if you choose. You can run 150 sets of factors. **ANY AND ALL EXPERIMENTS RUN WILL COUNT TOWARDS YOUR TOTAL.**

The project consists of two parts:

1.) **Design and conduct a cost-effective experimental program** for the pilot plant to determine the significant factors and optimal conditions for maximizing the production rate of the facility. Be sure to plan out the runs before you execute them in the pilot plant (online). Consider how many runs you will need to perform each step of the optimization.

2.) **Prepare a short report** *not to exceed 2 double-spaced pages* of text with a font size of 10 to 12 (images and tables can be included at the end of the report). The report should have three sections: 1) a discussion of the factor screening, 2) a discussion of the search for the optimum and 3) a section validating the assertion that you have reached the maximum. The search procedure should describe the experimental program used to find the optimal conditions. Finally, the sensitivity analysis should point out clearly which runs were used and how you were able to conclude that you are at the maximum production rate. The report can be broken down in the following format (please use headers and subsections as described below):

1. Factor Screening
   - Description of the screening design and explanation of why that design was used
   - Brief description of runs for screening. You do not need to include a listing of all your runs (the grader will have access to them), but you do need to indicate which runs were used for screening, optimization, and validation of the optimum.
   - Significant factors
2. Optimization
   - Description of the optimization design and why that design was used
   - Brief description of runs for optimization
3. Validation of the Optimum
   - Description of the validation design and why that design was used
   - Brief description of runs for validation
   - Analysis concluding that the optimum has been reached

The project will be graded out of 50 points: 35 points for your report (graded on content, quality, conciseness, readability) and 15 points for reaching 97% of your optimal value (calculated automatically based on your number of runs and maximum yield found).

Project Hints

- **Every group has a different problem, with a different maximum yield and different factor settings.** Any indications of plagiarism will result in significant reductions of points.
- **Complete and understand the labs on optimization before attempting this project.** You can practice with the labs, and *start over* as much as needed until you understand how this works before you use precious online runs that cannot be given back.
- The TAs and instructor are available for consulting on all questions relating to the use of JMP, the interface, as well as on general screening and optimization methodologies. However, you must independently make all decisions as to methods used, experiments run and interpretation of the results.
- There will be a penalty for using too many runs. Any run over 150 runs will cost you 0.5 points per run.
- There will be a bonus for using very few runs. You will receive 1 point for each run under 110 runs. However, this bonus will not be realized if you stop less than 3% from the optimum, and if you do not prove that the best point is an optimum.
- The penalty is usually greater for failing to reach the optimum than using a few extra runs…so don't stop too soon.

Project Assignment Memo

Following your graduation from Purdue you accept a lucrative job with the International Division of Maui-based SigMaui Squared Industries. Your first year with the company has been uneventful but satisfactory to both yourself and management. Your time has been consumed with lots of "training" and work on project teams. You avoided major confrontations with management and demonstrated a flair for improving various work processes. A problem has arisen in a newly acquired SigMaui Squared operations facility in Harristan. A relatively new French designed trans-esterification plant for producing Polyester (PE) Monomer has been unable to meet production quotas and has consistently failed to deliver the profits expected. The plant manager, "Big Jim" Washington, has been given responsibility for getting things "back on track". "Big Jim" calls your boss at Maui headquarters and asks that the best person possible be assigned to the task of improving plant performance. You are called into your boss's office and told to drop everything else and focus your attention on this problem. Big Jim has given assurances that the Harristan plant personnel will give you *carte blanche* in running any experiments you wish. However, both Big Jim and your boss, expect you to successfully optimize this facility within a month. Your mind paints visions of advancement in the company if you are successful. You express your gratitude for this opportunity to demonstrate your capability.

You leave the office feeling a little frightened but stimulated by the challenge. You check an atlas to see where Harristan is located. For some strange reason it is not in the company directory. Big Jim has assured you that terrorist threats are minimal and "most" employees return safely. You have your office professional arrange a meeting with the Harristani plant engineers for the next day, take the dog to the kennel, pick up a Berlitz guide to Harristanese and your passport, and catch a cab for the airport where you are booked on the 5:30 p.m. Blau Air flight to the Mean Squareport near the capital of Harristan.

Despite arriving at the production facility with a severe case of jet lag, you are eager to get started on the project. You ask the Harristani engineers to start off by giving you a tour of the facility and their assessment of the problem.

Description of the Trans-Esterification Plant

The engineers believe the bottleneck in the plant is the reaction step (no surprise). Two reactants Di-methyl-terephthalate (A) and Ethanol (B) undergo reaction in the liquid state and the presence of a liquid catalyst to produce the desired polyester monomer **B**is**H**ydroxy**E**thylterephT**h**alate (BHET) (C) and a volatile product Methanol (D) according to the reversible reaction

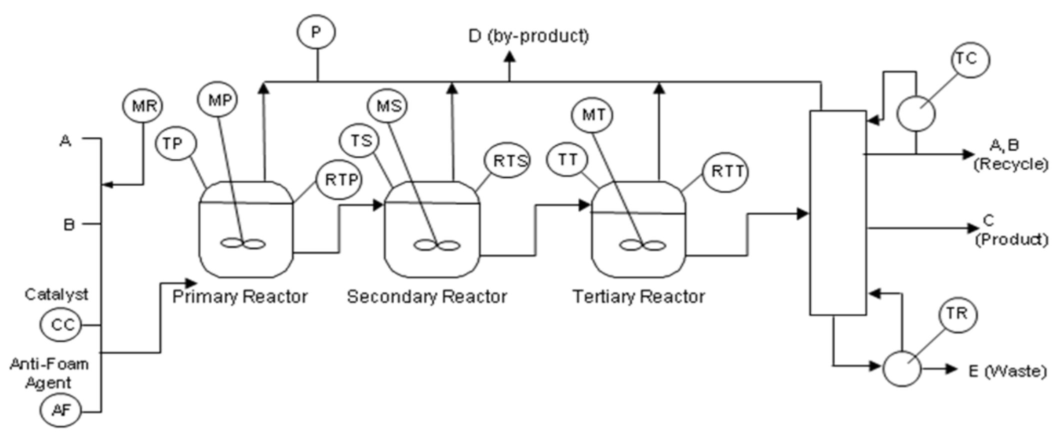
$A + B \leftrightarrow C + D$

In addition the reactants produce an undesirable by-product E.

$A + B \rightarrow E$

The impurity E not only consumes valuable raw material reducing the yield, but also must be removed from the reaction mixture for quality reasons and disposed of by incineration. The kinetics for the reaction are unknown. You naively ask why no kinetic information is available and are greeted with hostile stares. (You learn later that they have been trying to sell the idea of elucidating the reaction kinetics to SigMaui Squared management for months but were told it was too expensive). At any rate, now is not the time for research since you are under pressure to meet production demands and increase productivity as quickly as possible. The yield of BHET in the plant has been averaging 40% with day-to-day variations ranging from 20-80%. They have only vague ideas as to the reasons for the wide variation. Despite their best efforts using an informed search strategy, they have been unable to repeat the 80% value that was only achieved on one shift about two months earlier. It becomes immediately apparent that BHET yield is the key to improving process productivity. However, in selecting your response variable, you decide to use **daily production** (kg/day), which is calculated from yield because this is the only metric that seems to be important to SigMaui Squared Brass (not a musical group).

The following simplified flow diagram describes the process:



Process Flow Diagram

The Raw materials A and B are mixed together at a specified mole rate (MR) with the catalyst, CC, and an antifoaming agent, AF. The mixture is pumped to a fully mixed primary flow reactor, which is maintained at temperature, TP. The volatile product D separates from the reaction mixture. The level in the reactor controls the residence time in the reactor, RTP. The primary reaction effluent is fed to the secondary reactor, which is maintained at temperature, TS and residence time, RTS. The effluent from the secondary reactor is then fed to a tertiary reactor, which is maintained at temperature, TT and a residence time, RTT. The outlet from the tertiary reactor is fed to a splitter to separate the product C, by-product E and unreacted raw materials A and B for recycle. The product quality is controlled by the splitter condenser and reboiler temperature TC and TR receptively.

You ask the engineers to list the key factors they think have an effect on the yield and their operating range. The results are summarized in Table 1.

Table 1: Factors and their Operating Range

Descriptor	Meaning	Range
MR	A/B Mole Ratio of Reactants	(2/1 -7/1)
CC	Catalyst Concentration	(300-400ppm)
AF	Concentration of Antifoam Agent	(60ppm-80ppm)
TP	Primary Reactor Temperature	(250-270 °F)
MP	Primary Reactor Agitation Rate	(900-1500 rpm)
RTP	Primary Reactor Residence Time	(50min-75min)
TS	Secondary Reactor Temperature	(270-290 °F)
MS	Secondary Reactor Agitation Rate	(1200 -2000 rpm)
RTS	Secondary Reactor Residence Time	(40min-65min)
P	Reactor Pressure	(1-2 atmos)
TT	Tertiary Reactor Temperature	(290-310 °F)
MT	Tertiary Reactor Agitation Rate	(1000 -1600 rpm)
RTT	Tertiary Reactor Residence Time	(45min-60min)
TC	Condenser Temperature	(300 to 330 °F)
TR	Reboiler Temperature	(370 to 400 °F)

Unless you repeat runs the engineers believe that a change of at least 10% of the range of each of these factors would be needed at any part of the operating range to guarantee detecting a change in the response variable because of all the variability in the process. However, they are unwilling to even hazard a guess as to the magnitude of this variability.

Fortunately, there is a complete pilot plant facility available so that you can run experiments off-line without upsetting the actual process. Plant experience has shown that results from the pilot plant can be translated directly to the plant without scale-up difficulties. However, it takes a minimum of 4 hours to line out the pilot plant after changing any of the levels of the factors, and so the best you can do is obtain six runs a day if you work the operators 24/7. You also learn that the pilot plant is expensive. In fact they estimate it costs $5,000 per run in to cover raw materials, waste handling and staffing.