

Day 1 Homework Exercises

Smarter Experimentation for Chemists



Day 1 Homework Exercise

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Experiment one-factor-at-a-time

Your task is to optimise a simulated Heck reaction process using traditional trial-and-error or one-factor-at-a-time (“OFAT”) experimentation.

In JMP, open the file **Heck Reaction OFAT.jmp** (File > Open).

There are five factors: **Volume** of solvent, **Catalyst** amount, hold **Temperature**, hold **Time**, and **Sodium Acetate** amount. There is one response: **Yield** as a percentage.

Two trials or “runs” have been conducted. One with all factors set at the lowest extreme of their range, and one with all factors at the highest setting.

Conduct more runs with the aim of understanding how to maximise **Yield**. With each run you may only change the setting of one factor. The settings of all others must remain the same as for the previous run. Do not use factor settings outside of the range of the first two runs. Conduct as many runs as you like.

To conduct a run, enter settings in each factor column of a new row and click the green play button next to **Simulate Yield** in the top left of the table. Use Graph Builder to explore the data that you generate.

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Questions:

1. How does each factor affect the response, Yield?
2. What are the best settings of the factors to maximise Yield?
3. How many runs do you need to conduct to meet your objectives?

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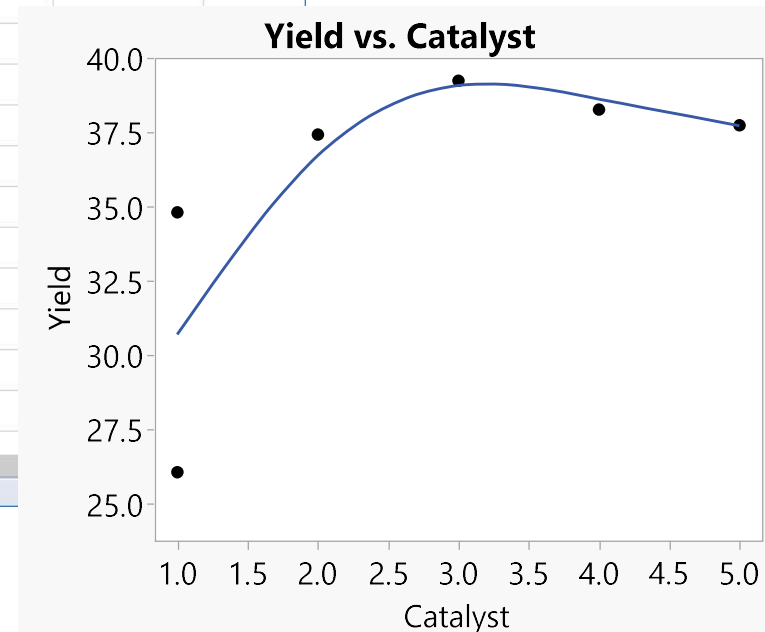
Heck Reaction OFAT - JMP Pro

	Volume	Catalyst	Temperature	Time	Sodium Acetate	Yield
1	1.5	1	50	4	1.5	26.0384983
2	10	5	120	24	4	37.7224787
3	10	4	120	24	4	38.2527456
4	10	3	120	24	4	39.2239579
5	10	2	120	24	4	37.4081982
6	10	1	120	24	4	.

Columns (6/0)
Volume ✓*
Catalyst ✓*
Temperature ✓*
Time ✓*
Sodium Acetate ✓*
Yield

Rows
All rows 6
Selected 0
Excluded 0
Hidden 0
Labelled 0

evaluations done



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Solutions:

There are no definitive answers for this exercise.

The important learning outcome is that experimenting in this way is open-ended, inefficient and ineffective.

You will most likely have found that with OFAT experimentation it is very difficult to meet your aims, or even to know whether you have.

In later lessons and exercises you will see how you can learn more effectively and efficiently using designed experiments.