

Lab exercise part 3: Building a model using multivariate regression

In Module 5a, once you determined the mathematical relationship between ϕ (the mobile phase mixture) and k (the retention factor), you could create your own model that predicted how the LC separation would behave for *any* mobile phase mixture, independent of the online simulator. In Module 5b today, you've used simplex optimization to try to find the best chromatographic separation while varying four GC parameters. But we haven't yet created a model, and after parts 1 and 2 of lab today you may not yet have a clear feeling for which of your GC parameters were most influential. So, creating a model is the next step – a model that will show how our separation depends on your four parameters, alone and in combination. We'll learn how to build such a model in class on Thursday, which will be led by experimental design guru Professor Lenny Perry from the School of Engineering.

The last task in lab today is to collect the input data that we'll need for building this model, so you have it ready to go on Thursday morning. We'll use the following process:

- A. For each of your four parameters choose two values ("levels") with your lab group.
 1. Parameter 1. _____ High = _____ Low = _____
 2. Parameter 2. _____ High = _____ Low = _____
 3. Parameter 3. _____ High = _____ Low = _____
 4. Parameter 4. _____ High = _____ Low = _____
- B. Now, splitting up the work with your lab group, you'll need to run a simulation with every possible combinations of High and Low values for the four parameters, and record the results. This experimental design is known as "factorial," because the number of experiments required is $(\# \text{ parameters})^{\# \text{ levels}}$, or $2^4 = 16$ in this case. Use the table below to ensure you get all 16 combinations and no repeats:

Parameter 1	Parameter 2	Parameter 3	Parameter 4	Response
high	high	high	high	
low	high	high	high	
high	low	high	high	
high	high	low	high	
high	high	high	low	
low	low	high	high	
low	high	low	high	
low	high	high	low	
high	low	low	high	
high	low	high	low	
high	high	low	low	
low	low	low	high	
low	low	high	low	
low	high	low	low	
high	low	low	low	
low	low	low	low	