Case Study

Teaching Chromatography Outside the Lab

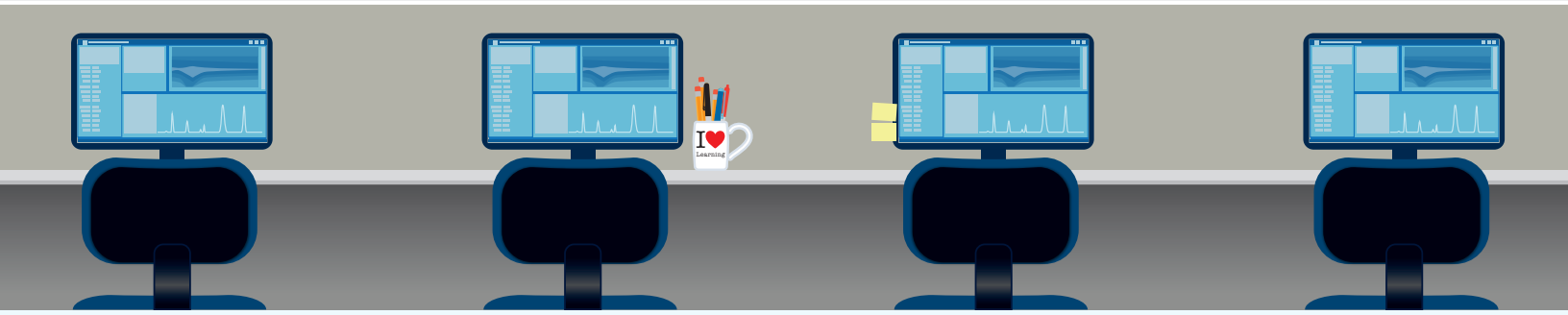
When lab equipment and time are limited, chromatography software fills the gaps

Industry: Academia

Purpose: Education

Software: ACD/Method Selection Suite

Highlight: A chemistry professor taught a virtual chromatography lab and coached his students to develop their own LC method using Method Selection Suite.



About Scott van Bramer

Dr. Scott van Bramer is a Professor and Chair of Chemistry at Widener University. He teaches several chemistry classes, including Instrumental Analysis and Environmental Analysis. Scott completed his PhD at the University of Colorado—Boulder.

Learn more about Scott at www.widener.edu/about/faculty-directory/scott-e-van-bramer.

Key Points

- Chemistry Professor Scott van Bramer used Method Selection Suite to teach virtual labs on LC method development
- LC simulations helped him explain difficult concepts to his students
- He helped his students learn through trial-and-error by seeing the results of changing chromatographic parameters
- They could change more parameters and run more experiments than they could in the lab

ACD/Labs

When experiment time is limited…

Students learn through experience and experiment.[1] They perform a task, reflect upon it and tie it to theoretical concepts, then put their knowledge to work in a new task. Hence hands-on labs help students turn chemistry lectures into chemistry understanding.

But labs are resource-consuming and difficult to scale. Equipment budgets are tight, expensive instruments are few, lab time is scarce, and instructors and TAs are stretched by a dozen demands. Even in normal times, these problems beset laboratory instructors, and the COVID-19 pandemic only increased the challenges.

How do you give students the trial-and-error experience of an experiment, the experience of making and learning from their own decisions, when labs aren't available at all? For Professor Scott van Bramer, the alternative—making up examples—was not appealing.

> "I was frantically trying to get my students some experience with chromatography. In particular, I wanted them to take a hand at experimental optimization, where they inject a real sample and look at the resolution and change the flow rate and mobile phase. I consider that to be an important learning step. And all of a sudden, I had nothing. I could just make things up and tell them, but that's really unsatisfying."

Software simulates the lab experience

He searched for a way to virtually simulate the lab experience. Though he found some web-based tools, "there wasn't really much going on there. There's not much depth to what I could do in terms of changing parameters for teaching."

Then he came across ACD/Method Selection Suite software. Method Selection Suite[2] is used by chemists worldwide to develop LC methods. More importantly for Scott, it includes a chromatogram simulator. Given a data set with chromatograms and the methods used to collect them, the simulator predicts how the chromatogram would look if parameters were changed.

How Scott used LC-simulation software with his class

Scott experimented with the sample data that comes with Method Selection Suite.

> "It took me a couple hours to see which variables I could change and figure out how to use the pre-loaded examples and look through them to find the most relevant ones. And then I played around with parameters to see what would come up with educationally useful changes—what ranges of parameters would make changes that [the students] could see."

About Method Selection Suite

ACD/Method Selection Suite helps chromatographers develop LC methods. It provides:

- Physicochemical-property prediction to help scientists understand how their analytes will behave
- pH- and column-selection tools to suggest good starting points for optimization
- 3D optimization to find the best method
- Simulated chromatograms, suitability-limit maps, and resolution maps to visualize results
- Retention-time prediction
- Boiling-point prediction for GC

To learn more about ACD/Method Selection Suite, go to https://www.acdlabs.com/methodselectionsuite.

[1] https://www2.le.ac.uk/departments/doctoralcollege/training/eresources/teaching/theories/kolb

[2] https://www.acdlabs.com/methodselectionsuite

Then, on a videoconference call with his students, he showed them the simulator. He worked with small groups, about six students at a time, so they could have better discussions. Students suggested changes to the method, and Scott ran the simulator to show them the results.

> "I would let them make choices about how we would change the solvent or gradient parameters, and how that would impact the resolution and retention times. There was a column-optimization tool, where we tried different columns and saw what would happen when you change the polarity of the column."

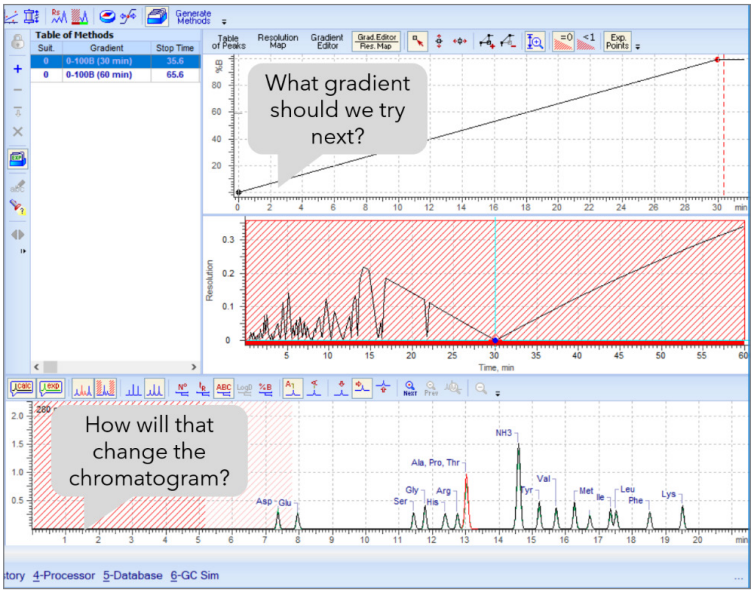


Figure 1. Students change the gradient and see the effect on the simulated chromatogram.

The surprising benefits of the virtual lab

Scott doesn't know how he would have taught his class without Method Selection Suite. "Honestly, at that point, I was stuck," he said.

Usually, his students learn method development in a day-long lab, working in shifts to design and refine a method. Though no software can replicate the hands-on part of that experience, Scott found a virtual way for his students to "make lots of decisions about the experimental design" and learn from the results.

And though a hands-on lab provides a more concrete experience, a virtual lab has its own benefits:

1. The students could change parameters that would be time-consuming or expensive to change in in-person labs, like particle size and column length.

   Normally, all we really change are the solvent parameters: the percent methanol and water or the gradient rate or the flow rate. That's all we can easily change.

   But with the simulator, we were able to change the column length. We could change the particle size, the packing materials. I don't have a half-dozen different columns in the lab and time to change them and let them equilibrate and then run an experiment.

2. The class could run more experiments, because each trial took a few seconds rather than tens of minutes.

   We were able to come up with a much more complicated, involved experimental design…because, you know, this simulation only took seconds as opposed to 20 minutes [if you were going to change the solvent gradient and rerun the experiment]. So you could get stuff faster.

3. Because the students could see many examples, they readily grasped difficult concepts, including resolution, Van 't Hoff plots, and the trade-offs between chromatographic parameters.

   But with the simulator, all of this theoretical stuff with Van 't Hoff plots, they're actually able to see how

that impacted the chromatogram. And so I thought that was much more effective than anything I've normally been able to do.

4. The undergraduate students got a glimpse of the software they might use in a future job—software they don't usually see until they enter the working world.

   I also thought it was pretty cool to have access to something that undergraduates wouldn't normally see and that they would never normally learn about until they started working for a big company.

If Scott had lab access and more prep time, he would probably collect his own training data. The usual lab experiment—measuring caffeine in coffees and energy drinks—is designed for students to readily connect the lab results to their lives, whereas Method Selection Suite's sample data reflects research priorities.

> *"If I did something like protein or peptide analysis, [the students] wouldn't have that sort of immediate connection to it, so I tended to stay away from that. But that's what a lot of the training sets were, and I get it, because that's what people are going to be doing in lab."*

But whatever the analytes, the lessons students learned remained the same.

Both online and on-campus

With Method Selection Suite, Scott could hold a virtual lab session to replace cancelled in-person labs.

> "I can't think of another possible way for [the students] to get at least some experience with experimental optimization and chromatography without getting them to do something like this."

But even when campuses open again, Scott thinks simulations could supplement the hands-on component. Before starting experiments, students could use software to "better understand the experimental parameters…and better think about how to optimize their experiment." Whether online or on-campus, virtual labs can help students draw connections between theory and practice.

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