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SIMIODE Systemic Initiative for Modeling
Investigations and Opportunities with Differential Equations

STUDENT VERSION
CHEMICAL REACTION DATA COLLECTION

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STATEMENT

Alex and Hayden had known each other all their lives, having both parents buying houses next to each other before they were born. They did chemistry merit badge in scouts and went to the same undergraduate schools and now were in the same chemistry PhD program with the same advisor - almost twins. However, each was different from the other - one into sports, the other classical music; one lived off pizza and burgers, the other was a strict vegetarian; one into on-line action games, the other into everything FaceBook and Tweeting all the time.

So while they took turns on the late shift in their professor's lab, sometimes they just hung out for the evening - Alex calling out for pizza and Hayden doing his tofu salad. This Thursday night their professor, Alyson, wanted to see if they could figure out how to back out parameters from a reaction. She said to them, "Ok. Here's what we're gonna do. I have compound A in this beaker and it decomposes slowly in the presence of catalyst Y. At 5:00 PM you are going to dump a fixed amount of A (in ng) into this large beaker and at the same time add a large amount of catalyst as well as begin a continuous stream of A (in ng) into the beaker. I want you to collect data on the amount of ng of A in the beaker using the MicroTell Reader, record it, form a mathematical model, and back out the parameters.

"No more than 8 hours of data collection ought to do it and since our AutoCollect device is in the shop I ask you to do it the old fashion way, sample at reasonable time intervals and just record the amount of compound A that the MicroTell Reader tells you." She said all this to them as she left at 4:30 PM for the day; she did this every day, exactly at 4:30 PM.

Alex and Hayden chatted about a few things, then returned to their favorite activities - Alex doing on-line gaming and Hayden doing FaceBook. Suddenly, Hayden jumped up and said, "Gotta go for a bit. Start without me and I'll be back to finish. I am going to Wally's." (Wally's was a

favorite vegetarian hangout near the campus). Whoosh, he was off. No consultation, no hint of his ideas on data collection, the model, the parameters, etc. Just gone!!

So Alex concocted this scheme which fit just right with his gaming strategy of "think fast and act faster" - hey, it got him campus Union Board championship last year! He would collect data every three minutes. By then Hayden would be back and they could mid-course correct if they needed to do something different. Hayden did not call back. Indeed, when Alex did get hold of him about an hour into the run he got, "Don't bother me now. I met this girl!" Later there was no answer on his cell phone. Hmmmmm!

We offer Alex's data pairs of amount of compound A at some point in time and then the amount of compound A exactly 3 minutes later, but never with any time of observations recorded. Would you believe?

Your job is to help him recover all his professor wanted him to do.

1. From the data offered in pairs, the amount of compound A in ng as first element of pair and the amount of compound A in ng exactly 3 minutes later as the second element of pair - but with no times offered - formulate a kinetic model of the reaction with the extraction. His professor believes it is either a first order or second order reaction with a constant stream of additional compound A coming in. She did not tell them at what rate, i.e., ng compound A/minute, the stream was, but she did say that the original amount of compound A in the beaker solution was 80.82 ng.
2. Confirm your model, estimate your parameters, and use your model to determine exactly when Alex did take these observations so he can fill in his data log on the experiment for his laboratory based studies.
3. Offer up some advice for Alex so that he has a better chance at success in graduate school.

Alex's Data

Here is Alex's data of the amount of compound A in ng in the beaker with data pairs for initial observation as first element in each pair and data for the observation made 3 minutes later as second element of each pair. There is no recorded data as to when he made these observations. However, as absent-minded and irresponsible as he was in recording time data, he was very diligent in noting that all data pairs are 3 minutes apart!

ng of Compound A at Start of 3 Minute Interval	ng of Compound A at End of 3 Minute Interval
80.82	93.29
143.24	155.48
227.14	238.88
303.84	314.91
387.60	397.74
465.94	474.99
503.28	511.74
517.58	525.81
549.79	557.46
595.05	601.90
627.01	633.25
664.33	669.78
673.80	679.05
695.15	699.93
730.42	734.41
737.34	741.17
746.11	749.73
774.98	777.89
795.67	798.07