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SIMIODE Systemic Initiative for Modeling Investigations and Opportunities with Differential Equations

STUDENT VERSION
CHEMICAL REACTION DATA COLLECTION

Brian Winkel
Director SIMIODE
Cornwall NY USA

STATEMENT

A tired chemistry graduate student, Karla, who really wants to play Magnate II on her computer with her buddies, is stuck on Friday night lab duty. Just before he leaves the lab late at 9:00 PM her advisor says, "I am going to set up an experiment involving first order reaction in Formula X which will run for about 6 hours and I wonder if you can collect the data because the AutoData device is on the fritz. This is important to me and I will return in the morning for the data which I need to write up for the Monday Departmental Seminar. You can start it whenever you want, but I need the data by 10:00 AM tomorrow morning. Just hit the START button on the apparatus. Immediately, the initial amount of Formula X in ng will be injected into the solution while the stirrer moves it uniformly through the solution. At the same instant a steady but constant amount of Formula X compound will be added to the beaker with my patented ChemInfuser. At all times the reaction takes place, consuming the Formula X compound. I want you to formulate a kinetics model and confirm my theories about the rate of reaction. Blah, blah, blah ... Thanks." Whoosh, he is out the door! He is dating another graduate student and she continues to wonder if she should say something to the chair of the department about that.

After finishing Round 4 on her game (Jeff, that turkey in Physics, is in the lead in housing sales in Chicago and she is determined to beat him this time) she turns to the experiment. "Let's see now," she says to herself. "I turn it on and then I note how much Formula X is in the reaction chamber and write out the time and amount. It looks like there is an initial dump of Formula X amount and concurrently ChemInfuser starts adding a steady but constant amount of Formula X over time. Was I supposed to know how much the initial dump was? Did he tell me the ChemInfuser rate or amount? Rats, I did not write them down when he was talking to me. Gotta learn to stay focused!"

She checked out the apparatus and notes that the sampler and display is the new Vectra model so this should be easy, for the display screen is easy to read from across the room where the Big Screen Monitor is hooked up to the high speed computer where she knows she is not supposed to do gaming, but cannot resist because of speed and monitor size. Besides, there is an alarm app on the computer and she can use it to prompt herself to pay attention to the display so she can get good data for her professor.

Here is what went on during the evening. She started the experiment by turning on the switch which began the initial dump, the stirrer, and the ChemInfuser. She noted in her log book that the initial amount of Formula X was 12.21 ng from her reading of the display. She then proceeded to turn on the coffee machine, for the night would be long and she needed to be alert. Wilson, that slime bucket, again, took the last cream container. After searching the cabinets for creamer stuff she resigned herself that she would have to drink it black. "All the better," she thought as it would help keep her awake.

"Oops, time to take some data," she thought and rushed across the lab to the display. It was at 9 minutes and 23 seconds from the start, she noted. She thought to herself,"Why don't I plan to take data every ten minutes as that would be a nice time interval – regular, small, and easy to add increments of 10 rather than, say, π"

So she waited until the display got to exactly 10 minutes - an amazing instrument which she could click on at increments of 1/100th of a second and it would give the actual amount in ng of Formula X to the 1/1000th of a ng and hold it on the screen for 30 seconds so she could jot it down in her log book. "Here we go," she thought. Tap! Lo and behold it really worked. 12.90 ng of Formula X in the container after exactly an initial 10 minutes of reaction and ChemInfuser action. "So," she thought, "the good professor has set this devise to add more Formula X than is lost in the reaction. Interesting."

She was on a roll and this equipment was so much better than her measly data collector she and her fellow grad students had to share in their lab/office. If only the AutoData device was working. She could just play her game all night and never even have to pay attention to the experiment. But, she knew she would have to break away from her game on a regular basis to collect the data - every ten minutes for the 6 hour duration! That meant she could comfortably have snack runs down to the department snack room and bathroom runs as needed, from drinking all that coffee!

She returned to the Big Monitor game console to negotiate a trade of the rundown apartment building she had long ago added to her portfolio in exchange for the potential she saw in the industrial size lot on the other side of town. Bingo, she found a seller, actually a trader, in Alyson who never liked potential, only current income generating properties. "So how did Alyson ever acquire this lot in the first place?" she wondered. "Probably, in a larger deal," she muttered to herself.

They made the deal and she went on to consider the location of the other property she was considering, because it had proximity to the Metro line, but exactly how close ... and what about the schools ... "Oh my gosh, the experiment," she screamed at herself. Upon checking the display she found that it went into sleep mode and had to be tapped to bring up the full display. "Oh that

smarts for me." She was thinking she might now have to really pay attention to the display, maybe even note the time on the browser at the big Monitor machine where she sat for her gaming.

She had not realized how much time had passed. She noted the amount of Formula X as 15.73 ng. "I better pay close attention here, at least at the start. So I will check the apparatus for connections and wiring and just stay on this side of the lab until another ten minute interval passes and note the amount of Formula X." Bingo, at exactly 10 minutes from the previous recording she noted the amount of Formula X was 16.26 ng. "Continuing to increase," she noted.

Meanwhile, the game got intense with seven folks from Europe joining in during her wee hours of the morning - and they were sharp traders, so she became more and more absorbed in her game ... forgetting to collect data on a regular basis, time and time again!

Well, as one might imagine, Karla was not the most disciplined laboratory person, so this whole procedure of NOT paying attention to the display, running to record the amount of Formula X, and then telling herself she MUST do better while waiting exactly 10 minutes and getting another reading, only to forget after that and come back, who knows how much later, to get another reading with her 'contrite, but really not reformed effort, in taking readings, some time later in the experiment, again followed by the reading exactly 10 minutes later. It went on and on for almost 6 hours.

Here is the amazing part. Karla never once recorded the actual time of her observations in her log book, just the amount of Formula X, noting which was the first of her two, separated by 10 minutes, observations, over and over, throughout the night. It was simply amazing (and regrettable) that she did not record the actual time of ANY observations, except the first two at time $t = 0$ min and $t = 10$ min.

We offer her data pairs of amount of Formula X at some point in time and then the amount of Formula X exactly 10 minutes later.

Your job is to help her recover all her professor wanted her to do, by developing a mathematics model, estimating parameters, solving the model, and confirming that her data and the model conform.

1. From the data offered in pairs, the amount of Formula X in ng as first element of pair and the amount of Formula X in ng exactly 10 minutes later as the second element of pair, and the knowledge that this was a first order reaction in Formula X with a steady but constant infusion of Formula X into the beaker formulate a kinetic model of the reaction with the extraction. Alas, Karla's data offers no time of observation except for the first two observations at time $t = 0$ and $t = 10$ minutes.
2. Confirm your model, estimate your parameters, and use your model to determine exactly when Karla did take these observations so she can fully fill in her data log on the experiment.
3. Offer up some advice for Karla so that she has a better chance of surviving in graduate school.

Karla's Data

Here is Karla's data of the amount of Formula X in ng in the beaker with data pairs for the initial observation as first element in each pair and data for the observation made 10 minutes later as second element of each pair. There is no recorded data as to when she made these observations.

ng of Formula x at Start of 10 Minute Interval	ng of Formula x at End of 10 Minute Interval
12.21	12.90
15.73	16.26
16.32	16.84
18.22	18.65
20.04	20.39
21.49	21.78
22.76	23.01