Supporting Information for

Remote Learning of COVID-19 Kinetic Analysis in a Physical Chemistry Laboratory Class

Kelle D. Hart, Chelsea Thompson, Clay Burger, Dylan Hardwick, Amanda H. Michaud, Abdul H.M. Al Bulushi, Cole Pridemore, Carson Ward, Jixin Chen*

Department of Chemistry and Biochemistry, Ohio University, Athens, Ohio

chenj@ohio.edu

SI 1. Prelab preparation for COVID-19 Data Analysis

- We will do the COVID-19 data searching and analysis during lab time.
- Please check if you have installed **Microsoft Excel** or have access to the Google spreadsheet service during the lab.
- Please watch the following videos before coming to the lab:
- https://medicine.yale.edu/coved/modules/covid/challenge4/
- https://www.youtube.com/watch?v=Kas0tIxDvrg

Your final reports will look something like the sections listed below.

Introduction

In this lab, we will first have a very brief background introduction of COVID-19, kinetic models in the literature for infectious disease, and motivation of the analysis (e.g. understanding R_0, and its correlation with social regulations). Then we will start with a calculation on a typical mortgage model to practice the modeling technique. Then we will use the suspected-infectious-recovered (SIR) model to fit the COVID-19 data of a few states. SIR model is a commonly used kinetic model for infectious diseases spreading.

Methods

We will use Excel spreadsheets to numerically simulate kinetic models in the lab. Use the models, we will guess the parameters using manual regression method to obtain a fit of the data.

Protocol

Simulate a fixed payment mortgage plan, using a compound interest and payment model.

Search the reliable online database to find out the COVID-19 confirmation and other hidden parameters such as incubation time, lifetime, and death rate…

Choose a reaction model that the R0 value is the only or major parameter to adjust.

Come up with an excel file to plot the data, and co-plot the model on top of the data. Then adjust the R_0 value to get a rough overlap of the two sets of data.

Fit the first 2 weeks of data for the initial R_0.

Plot dC/dt to identify the turning points of the data (waves of COVID).

In each part of the time window guess the best R_0.

Try to correlate possible social events with each spike or reduction of R_0.

Simulate the future trajectory for different conditions including, reducing 30% social interactions, social distancing (6 feet assuming 50% reduction of *k*), face mask (assuming 90% population and 60 reductions of *k*), and vaccine (assuming a steady increase in two years to full coverage).

Come up with any slightly different model to fit the Ohio data. (optional)

Results

Explain the results of mortgage simulation with fast pay, fixed pay, and underpay.

Give a scheme of the model and explain your model.

Plot data and your best fit.

Plot R_0 over time and try to correlate it with major social events, e.g. lockdown, mask order, holiday, reopen…

Plot possible future trajectories with different regulations.

Discussion

Compare the models.

Discuss the data and draw some conclusions.

Conclusion and Perspective

Conclude the effect of social distancing, mask, and vaccine. Comment how realistic is the mathematic model.

References

Search the scientific literature using google scholar or our professional search engine and cite them in your report.

SI 2. Lab report grading and format instruction

Instruction for lab report	Total 100 pts
Title and Abstract	10 pts
Introduction	20 pts
Experimental Section	10 pts
Results	40 pts
Raw data in tables	
Processed major results in tables or graphs	
Describe the results	
Discussion	10 pts
Conclusions	5 pts
Reference	5 pts

Double-space. Font: Arial (12) or Times (12). Margins 1" on four sides.

CHEM 4540L: Physical Chemistry Lab Report

Lab 1. COVID-19 kinetic analysis

xxxxx, xxxx@ohio.edu, mm/dd/yyyy

(your name along with the email address, and date of the report)

Lab partner: xxx, xxx, … TA name (if any): xxx, xxx

Experiment 1: (Title)

(here you come up with a title to best describe your experiments or your conclusions <20 words).

Abstract (<250 words)

1. Motivation
2. Problem to address
3. Method
4. Main findings/observations. Quantitatively describe your observations. E.g. the quantum yield of the dye is measured to be 60±5% at 298 K in water.
5. Major conclusions.

One sentence (or two) to most of these points.

Introduction (Literature review)

One- to three-page, 4-6 paragraphs describing the motivation, background, gap of knowledge (optional), problems to address, experimental methods in the literature, and this experiment.

Note: in your own words with appropriate citation given. For example, the melting and annealing of DNA hairpins are essential in many biological processes such as

replication, transcription, recombination, gene expression, and DNA transposition for both prokaryotic and eukaryotic systems.[1]

Citations can be managed with free software such as Mendeley or others.

Experimental section

Describe the reagents, instrumentations, and protocol to carry out the experiments. The section should be precise and should contain everything about the experiments for the others in the field to reproduce the results and analysis (with no problem emailing you for details). Sometimes data treatment methods also go into this section. Safety concerns need to be reported here.

Results

Data obtained are listed in the order you think is good for the readers to follow to solve the questions you have raised in the introduction section. These results should lead to conclusions to solve the problems. Format of a table:

Table xxx. (Title)

Table body

Table notes

e.g.

Table S1. Fitted rate constants of simulated data.[a]

k (s^{-1})		Initial states		
		1	2	3
Final states		Non-binned 1 ms, noise-free		
	1	0	1.5±0.1	2.5±0.3
	2	0.5±0.1	0	3.0±0.2
	3	1.1±0.1	2.1±0.2	0
		Non-binned 1 ms, noise added		
	1	0	99±2	8.1±0.3
	2	31±0.6	0	35±1.0
	3	6.1±0.3	90±2	0
		Binned at 10 ms, noise-free		
	1	0	1.6±0.2	1.4±0.2
	2	1.1±0.1	0	4.3±0.2
	3	0.5±0.1	2.1±0.2	0
		Binned at 10 ms, noise added		
	1	0	1.6±0.2	1.4±0.2
	2	1.1±0.1	0	4.3±0.2
	3	0.5±0.1	2.1±0.2	0

[a]Standard deviations are from 10 simulations.

Format of a figure/graph/diagram/plot:

Figure body (width ~3.5” or width ~ 7”)

Figure xxx. (figure caption describes the meanings of each part)

e.g.

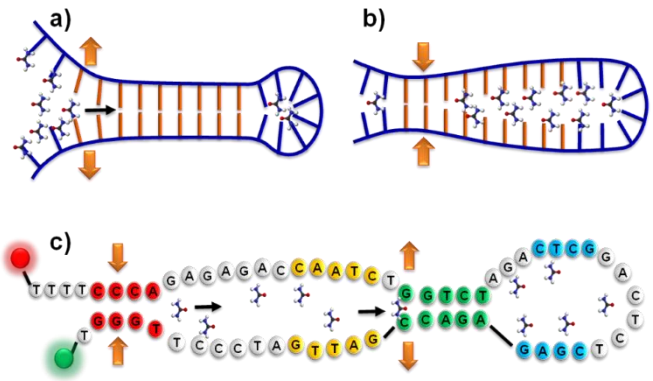

Figure S1. Schematic of proposed examples of unfolding/folding routes of (a, b) model DNA hairpins and (c) the TAR-DNA hairpin with two dyes Cy3 and Cy5 labeled to the ends. The small molecules represent the solution, and the double helix is not shown for easier demonstration.

Explain the meaning of the results and list the equations to obtain these results.

Use Powerpoint, Excel, and free fitting software.

Discussion

Describe the questions and answer all the questions with your data. Sometimes you can compare your results to the literature or use literature results to support the discussion. Cite appropriately.

Conclusions

Similar structure as the abstract with an emphasis upon your results and conclusions. No words limit but usually concise.

References

(ACS style, free software Mendeley choose style “The Journal of Physical Chemistry B”)

(1) Watts, J. M.; Dang, K. K.; Gorelick, R. J.; Leonard, C. W.; Bess Jr, J. W.; Swanstrom, R.; Burch, C. L.; Weeks, K. M. Architecture and Secondary Structure of an Entire HIV-1 RNA Genome. *Nature* **2009**, *460*, 711–716.

Tips.

One topic in each paragraph with the first sentence states the major conclusions or topic of the paragraph. So one can just read the first sentence to get the idea of the whole story.

- Use scientific reporting methods:

  SI units

  Significant figures

  Standard deviations

  Error propagations

  Least square/regression analysis/fitting

- Check for all tables, figures, graphs, plots, and spectra:

  Titled and numbered

  Clearly named and labeled

  Everything is discussed in the text body (don't show the data that are not needed)

  Right size

- In experimental section cover

  Relevant formulas

  Sample calculations

  Error propagations

- Include in the results section

  Final results with an estimated uncertainty

  Compare with the literature values if there are. If not estimate the accuracy either theoretically or with something similar in the literature.

- Include in the discussion section:

  The meaning/significance of the results

  Evaluate the data quality

  Error analysis

- Double-check the quality of the report

  Structure organization/logic story flow

Clarity

Spelling

Grammar (use Grammarly free service to check grammar)

Unfinished discussions