

Problem Set 2

- You may use your course materials and/or any literature resources (as well as the internet) to formulate your solutions.
- You may work in teams. All model/analysis code must be submitted to GitHub and the link submitted to the teaching staff email. Each student on the team must be a collaborator on the GitHub repository.
- Problem Set 2 is due on **Thursday, March 4, 2021 by 11:59 PM.**

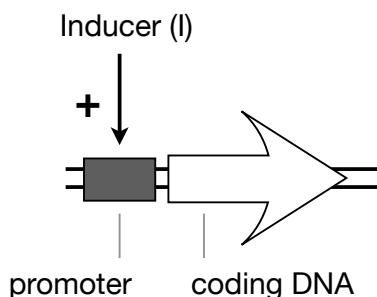


Figure 1: Inducer I induced expression of gene G in the myTXTL *E. coli* cell free expression system.

Consider inducer I induced expression of gene G in the myTXTL *E. coli* cell free expression system at $T = 37^{\circ}\text{C}$ (Fig. 1). Develop a simulation of the steady-state mRNA concentration as a function of the concentration of inducer I . Initial model code for this simulation is available at: <https://github.com/varnerlab/CHEME-5440-7770-PS2-S21.git>. The teaching team needs your help completing this code.

Assume: (i) The cell free reaction is well mixed with a constant volume $V_R = 15\mu\text{L}$; (ii) The length of gene G is $\mathcal{L} = 690$ nt; (iii) The concentration of G is 5nM and constant; (iv) Parameter values can be obtained from Adhikari et al (2020) Front. Bioeng. Biotechnol. <https://doi.org/10.3389/fbioe.2020.539081>, Garamella et al (2016) ACS Synth Biol 15:344-55 doi:10.1021/acssynbio.5b00296 or other sources such as BioNumbers; (v) treat I as σ_{70} when looking up parameters.

1. Fill in the missing parameters values in the `Parameters.toml` file in the config directory.

2. Compute any missing values in the `Problem.jl` file in the `src` directory. Make sure to add these values to the problem dictionary (they are used in other parts of the program).
3. Complete the implementation of the kinetic limit of transcription of \mathcal{G} , denoted by $r_{X,\mathcal{G}}$, in the `Kinetics.jl` file in the `src` directory.
4. Complete the implementation of the transcriptional control variable $\bar{u}(\dots)$ in the `Control.jl` file in the `src` directory. Describe the promoter using a three state model with states; 1: bare DNA, 2: RNAP bound to promoter, and 3: Inducer and RNAP bound to promoter. State 2 and 3 lead to expression. Describe the binding of inducer I to the promoter with the hill-type expression:

$$f_I = \frac{I^n}{K_D^n + I^n} \quad (1)$$

5. After completing steps 1 - 4, the model code should be complete. Execute the `execute_me_PS2.jl` script to produce a plot of inducer concentration versus steady-state mRNA concentration.

Submit the figure generated by the `execute_me_PS2.jl` to the teaching team email for full credit on PS2.