SAMPLE PROBLEM PROPOSAL (SENIOR), 2022

Singapore International Modelling Challenge

v0.1

Sample Problem Scope

This sample problem gives an illustration of the type of questions to be expected in the main challenge. The challenge problem will resemble the logical flow here, with a similar mix of mathematics, modelling and computation. However, the subject matter, breadth and depth of the challenge problem will be different from this sample.

Sample Challenge Problem

In this sample challenge, we investigate the dynamics of a catalytic reaction on a surface. We would like to remove a harmful substance X from the atmosphere. A catalytic surface is used for this purpose. The surface contains N total reaction sites. Each X molecule can adsorb onto an empty site S to form a complex XS. The complex XS then diffuses quickly across the surface, and when it meets another site complex a reaction may occur to produce X_2, a harmless product. This also frees the two sites, which will become available for adsorption afterwards. Figure 1.1 gives an illustration of this process.

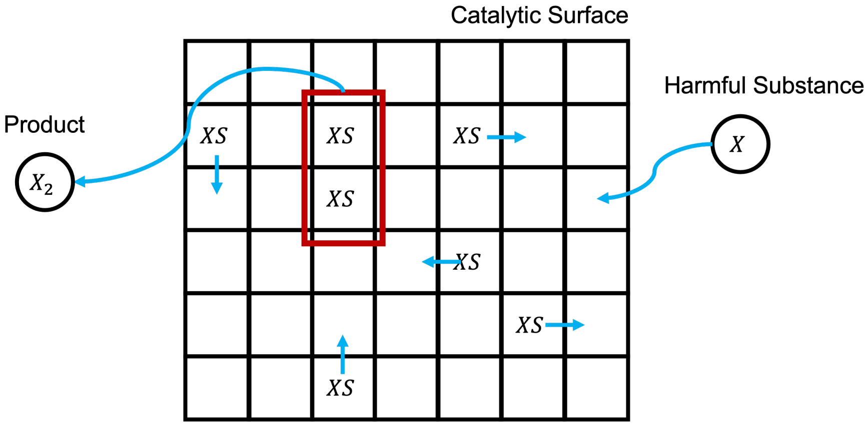

Figure 1.1: Catalytic Reaction on a Surface.

We may also write the reaction equations as follows:

$$X + S \longrightarrow XS \tag{1.1}$$

$$2XS \longrightarrow 2S + X_2 \tag{1.2}$$

1.1 A Stochastic Process Model

Let us first explore a stochastic model for this catalytic process. We index the observation times by a discrete sequence $t = 0, \Delta t, 2\Delta t, \dots,$ where $\Delta t > 0$ is the time step. Let us denote by $N_{XS}(t)$ the number of occupied sites (XS) at time t. The number of empty catalytic sites is thus $N_S(t) = N - N_{XS}(t)$.

In each time step $t \mapsto t + \Delta t$, exactly one of the following happens:

- N_{XS} increases by 1 due to adsorption of X onto the surface (Eq. (1.1)). This occurs with probability proportional to $N_S = N - N_{XS}$. This is assuming that the ambient concentration of X is held constant by a reservoir. Set this probability as $P_1 = a\Delta t(N - N_{XS})$, where $a > 0$ is a constant and Δt is sufficiently small so that $P_1 < 1$.
- If $N_{XS} \geq 2$, N_{XS} decreases by 2 due to reaction of two occupied XS sites (Eq. (1.2)). This occurs with probability proportional to $\binom{N_{XS}}{2} = \frac{1}{2}N_{XS}(N_{XS} - 1)$, since this is a bi-molecular reaction. Here, we are also assuming that the diffusion of XS on the surface is rapid, so that the system is well-mixed. We set this probability as $P_2 = \frac{1}{2}b\Delta t N_{XS}(N_{XS} - 1)$, where $b > 0$ and Δt is sufficiently small so that $P_2 < 1$.
- Nothing happens, and N_{XS} remains the same. This occurs with probability $P_3 = (1 - P_1 - P_2)$, and we assume that Δt is sufficiently small so that $P_3 > 0$.

(a) Write a programme to simulate the evolution of $N_{XS}(t)$ starting from the initial condition $N_{XS}(0) = 0$ and $a = 1.5 \times 10^{-3}$, $b = 2.5 \times 10^{-5}$, $\Delta t = 0.1$, $N = 100$. Plot your simulation results for $N_{XS}(t)$ up to $t \leq 10$, for 5 separate runs.

(b) The *steady state distribution* for this process is the distribution of $N_{XS}(t)$ for large/infinite t. Equivalently, it is the distribution of N_{XS} which does not change in time under the process above. Plot an estimated steady-state distribution for N_{XS} with parameter settings in (a). You may use your simulation, or other means to compute this distribution.

(c) How does this distribution change as N is increased?

1.2 A Differential Equation Model

As seen previously, the stochastic process model may be unwieldly for analysis. A popular alternative to model the kinetics of chemcial reactions is using differential equations. Instead of the number of occupied sites, we can monitor the proportion of occupied sites $c(t) = N_{XS}(t)/N$. By taking the formal limit $N \longrightarrow \infty$, we can regard $c(t)$ as a real number. Moreover, we can take $\Delta t \longrightarrow 0$, which gives rise to a continuous-time evolution model for $c(t)$:

$$\frac{d}{dt}c(t) = \alpha(1 - c(t)) - \beta c(t)^2, \qquad \alpha, \beta > 0 \tag{1.3}$$

The first term on the right hand side models reaction (1.1) and the second term models reaction (1.2).

(a) Solve the equation (1.3) with initial condition $c(0) = 0$ and parameter values $\alpha = 0.3, \beta = 0.5$. Either analytical or numerical solutions are accepted. Plot $c(t)$ vs t for $t \in [0, 10]$.

(b) Suppose we have an ambient sensor that monitors the concentration of the product chemical X_2 from reaction (1.2) as a function of time. Let us call this quantity $c_{X_2}(t)$. Suppose that we observe that $c_{X_2}(t)$ approaches a straight line $c_{X_2}(t) \approx pt + q$ for large t, where $p, q > 0$. Our goal is to estimate the constant α (related to the ambient concentration of the harmful chemical X) from this information, assuming the constant β is known. Devise a method to do this.

1.3 Data-Driven Modelling of Reaction Mechanisms

For complex reactions, the reaction mechanism is often unknown. In this case, we can make use of data-driven methods to model the evolution of a surface-catalysed reaction.

You are now provided with a dataset containing the following content (saved in JSON format):

```
data
 |__train.txt
 |__test.txt
```

The training data contains records from 50 simulated temporal trajectories of the following 3 quantities:

- $c_X(t)$: concentration of the harmful chemical X
- $c_{XS}(t)$: coverage of the catalytic surface by XS complex
- $c_{X_2}(t)$: concentration of the harmless product chemical X_2

The test dataset contains 10 unseen initial conditions of $c_X(0), c_{XS}(0), c_{X_2}(0)$.

(a) Predict the trajectories of $c_X(t), c_{XS}(t), c_{X_2}(t)$ starting from the initial conditions given in the test dataset. You should explain clearly how your predictive model is built.

(b) Infer a likely catalytic reaction mechanism and explain how you arrived at it.