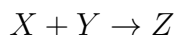


WORKSHEET: COMPUTING WITH CHEMICAL REACTIONS

MATH 185 - HOW TO BE A MATHEMATICIAN

A test tube contains molecules of several types, called *species*, which we label X , Y , Z , and so on. A *reaction* is a rule for changing the contents of the tube. The reaction



can happen whenever the tube contains at least one X and at least one Y . When it happens, one X and one Y are removed and one Z is added. The reaction $2X \rightarrow Y$ can happen when the tube contains at least two X 's, and it replaces two X 's by one Y . The symbol $\emptyset$ means “nothing,” so $X + Y \rightarrow \emptyset$ removes one X and one Y and adds nothing.

A list of reactions is called a *reaction network*. The tube follows two rules.

- At each step, any reaction that is able to happen might be the one that happens. You do not get to choose which one.
- The process stops when no reaction is able to happen.

Example. The network is $X + Y \rightarrow Z$, and the tube starts with 2 X 's and 3 Y 's.

	X	Y	Z
start	2	3	0
after step 1	1	2	1
after step 2	0	1	2

After step 2 there are no X 's, so the reaction cannot happen and the process stops.

Part 1: Find what is in the tube when the process stops.

- (1) The network is $X \rightarrow Y$. The tube starts with 5 X 's. What is in the tube when the process stops?
- (2) The network is $2X \rightarrow Y$. The tube starts with 7 X 's. What is in the tube when the process stops? If the tube starts with x molecules of X , how many Y 's are there at the end, and how many X 's?
- (3) The network is $X + Y \rightarrow Z$. The tube starts with 4 X 's and 6 Y 's. What is in the tube when the process stops? If the tube starts with x molecules of X and y molecules of Y , how many Z 's are there at the end?
- (4) The network has two reactions, $X \rightarrow Y$ and $X \rightarrow Z$. The tube starts with 3 X 's. List every possible content of the tube when the process stops.

- (5) The network is $X \rightarrow X + Y$. The tube starts with 1 X . What happens?
- (6) The network has two reactions, $X \rightarrow 2Y$ and $Y + Z \rightarrow \emptyset$. The tube starts with 3 X 's and 4 Z 's. What is in the tube when the process stops? Can a different order of reactions give a different answer? Explain your reasoning. Then answer the same questions when the tube starts with 2 X 's and 5 Z 's.

Definition. Put x molecules of X in the tube and nothing else (or, for a function of two numbers, x_1 molecules of X_1 and x_2 molecules of X_2). A reaction network *computes* the function f if, for every starting input and every order in which the reactions happen, the process stops, and when it stops the tube contains exactly $f(x)$ molecules of Y (or $f(x_1, x_2)$ molecules of Y). For example, the network $X \rightarrow Y$ computes $f(x) = x$.

Part 2: Design networks that compute given functions, and prove that they work.

- (7) Design a network that computes $f(x_1, x_2) = x_1 + x_2$.
- (8) Design a network that computes $f(x) = 2x$.
- (9) Design a network that computes $f(x) = \lfloor x/3 \rfloor$, the number $x/3$ rounded down.
- (10) The function $f(x_1, x_2) = x_1 - x_2$ makes sense as a count of molecules when $x_1 \geq x_2$. A student proposes the network with two reactions $X_1 + X_2 \rightarrow \emptyset$ and $X_1 \rightarrow Y$ to compute it. Find starting counts with $x_1 \geq x_2$ and an order of reactions for which the tube ends with the wrong number of Y 's.
- (11) Design a network that computes $f(x_1, x_2) = x_1 - x_2$ whenever $x_1 \geq x_2$. Explain why it works. (Problem 6 may help.)

- (12) Show that the network $X_1 + X_2 \rightarrow Y$ computes $f(x_1, x_2) = \min(x_1, x_2)$ for every x_1 and x_2 . *Hint:* When the reaction happens, what happens to (number of X_1) - (number of X_2)? What happens to (number of X_1) + (number of Y)?
- (13) Design a network that computes the function with $f(x) = 1$ when x is odd and $f(x) = 0$ when x is even.
- (14) Design a network that computes the function with $f(x) = 1$ when $x \geq 1$ and $f(x) = 0$ when $x = 0$.
- (15) Design a network that computes $f(x_1, x_2) = \max(x_1, x_2)$. *Hint:* $\max(x_1, x_2) = x_1 + x_2 - \min(x_1, x_2)$.

Part 3: Find functions that no network computes.

(16) Explain why no network computes $f(x) = x + 1$. *Hint:* Consider $x = 0$.

(17) Try to design a network that computes $f(x_1, x_2) = x_1x_2$. Why does the network $X_1 + X_2 \rightarrow X_1 + X_2 + Y$ fail?

Mathematicians have proved that no reaction network computes $f(x_1, x_2) = x_1x_2$.¹ They have also described exactly which functions reaction networks can compute.

¹H.-L. Chen, D. Doty, and D. Soloveichik, *Deterministic function computation with chemical reaction networks*, Natural Computing **13** (2014), 517–534.