MATH 448 — Worksheet: Computing with Chemical Reactions

Name: _____

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

$$X + Y \to Z$$

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 $2X \to Y$ can happen when the tube contains at least two X's, and it replaces two X's by one Y. The symbol $\varnothing$ means nothing, so $X + Y \to \varnothing$ 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 $X + Y \to Z$, 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 $X \to Y$. The tube starts with 5 X's. What is in the tube when the process stops?

(2) The network is $2X \to Y$. 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 $X + Y \to Z$. 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, $X \to Y$ and $X \to Z$. The tube starts with 3 X's. List every possible content of the tube when the process stops.

(5) The network is $X \to X + Y$. The tube starts with 1 X. What happens?

(6) The network has two reactions, $X \to 2Y$ and $Y + Z \to \varnothing$. 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 $X \to Y$ computes $f(x) = x$.

Part 2: Design networks that compute given functions.

(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.