Complex Chemical and Biochemical Reactions: Maybe Fuzzy Techniques Can Help

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Abstract Chemical reactions are usually described by equations of chemical kinetics, where the reaction rate is proportional to the product of the concentration of the interacting molecules. Such equations have been thoroughly studied. However, in many practical situations, e.g., in biochemistry, chemical reactions are strongly catalyzed, in which case the reaction rate is proportional to the minimum of the concentrations. Such equations are much less studied in chemistry, so it is reasonable to looks for other areas where similar equations appear. One such area is fuzzy techniques, so we hope that fuzzy techniques can help when analyzing such complex chemical and biochemical reactions.

1 Chemical reactions are important

Chemical reactions are ubiquitous:

- They are important on geosciences, where they affect long-term changes.

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- They are important in biology: all our activities are chemical reactions.

In general, chemical reactions are described by equations of chemical kinetics. In these equation, the rate of a reaction

$$A + B \to C$$

is proportional to the product $a \cdot b$ of concentrations a and b of the interacting substances.

2 Where the usual chemical kinetics formula comes from

The formula $a \cdot b$ makes perfect sense. Indeed, the reaction rate is equal to the sum of the rates corresponding to each spatial location.

For each location, for the reaction to happen, you need to have two molecules meet there. The probability that molecule A gets there is proportional to its concentration a. The probability that molecule B gets there is proportional to its concentration b.

These two events are usually independent. So, the probability that both molecules get there is equal to the product of these probabilities. Thus, the rate is indeed proportional to the product of the concentrations $a \cdot b$.

3 The resulting reaction is often very slow

The problem with the usual formula $a \cdot b$ is that when a and b are small, the reaction is very slow.

- When students mix two chemicals in the lab, it takes seconds – or even minutes – for the reaction to finish. (The only exception is when everything accidentally blows up – a disaster.)
- In contrast, we sometimes need to react in a few milliseconds.

Living creatures need to react fast in order to survive.

4 How can we speed up chemical reactions

Evolution came up with a way to speed up these reactions. (By the way, chemical engineering uses the same ideas to speed up industrial chemical processes.) The idea is to concentrate both molecules in a small volume – for example, on a surface of a catalyst.

When in an area, concentrations are high, there is no randomness left. Molecules are all there, so they can start interacting right away.

Let us illustrate this on a similar example – predator-prey equations. In general, the rate with which wolves eat rabbits is proportional to the product of their concentrations. The reason for this is the same as for chemical reactions: we need rabbits and wolves to meet at the same point. However, if you place wolves and rabbits in the same small space, the situation is different. Wolves can start eating rabbits right away. Each wolf start eating a rabbit – as long as there are enough rabbits. In general, the rate if this reaction is proportional to the minimum of the two concentrations.

Similarly, for high-concentration chemical reactions, the reaction rate is proportional to $\min(a,b)$.

Sometimes, the speed up is not complete. In this case, the reaction rate $r(a,b)$ is larger that $a \cdot b$ but still smaller than $\min(a,b)$.

5 How is all this related to fuzzy logic

When we go from slow to fast reactions, we replace product with min. In chemical kinetics, there was not much research on such reactions. It is thus desirable to look for other areas where a similar replacement has been analyzed.

There is one research area where one of the main ideas is using min and other functions instead of the product. This idea is fuzzy logic; see, e.g., [5, 6, 7, 8, 9, 10]. In fuzzy logic, such situations have been thoroughly studied. It is therefore reasonable to apply fuzzy techniques and fuzzy intuition to chemical reactions as well.

6 From simple to more realistic chemical reactions

In chemical engineering, we are usually interested in a single chemical reaction. For example, we may be interested in transforming oil molecules into some useful chemical.

In contrast, for a living cell to function, a lot of different reactions have to take place. Let us consider a complex – but still somewhat simplified case – when we have several reactions

$$A_i + B_i \to C_i.$$

7 How to describe such reactions in biological setting

How can we describe such systems of reactions in biological setting? We start with some concentrations a_i of A-molecules and concentrations b_i of B-molecules

Evolution leads to optimal setting. In particular, the catalytic surface is made exactly the size needed for all the reactions. Otherwise, we would waste resources on a useless surface.

So, the sum of all A-concentrations should be exactly the amount needed for all the reactions. To make our analysis simpler, we can change the measuring unit for measuring concentrations. For an appropriate unit, the sum of concentrations becomes 1:

$$a_1 + \ldots + a_n = 1.$$

In other words, we consider *relative* concentrations.

Similarly, concentrations of B-molecules add up to 1: $b_1 + \ldots + b_n = 1$. After all the reactions, the concentration of each C-molecule is equal to $\min(a_i, b_i)$. So, the relative concentration of all C-molecules takes the form

$$c_i = \frac{\min(a_i, b_i)}{\sum\limits_{j=1}^{n} \min(a_j, b_j)}. \quad (1)$$

For a general reaction rate formula $r(a,b)$, we have a more general expression

$$c_i = \frac{r(a_i, b_i)}{\sum\limits_{j=1}^{n} r(a_j, b_j)}. \quad (2)$$

8 Let us describe all this in fuzzy terms

How can we describe this in fuzzy terms?

For high-concentration reactions with rate $\min(a,b)$, we interpret a and b as degrees of confidence that we have A and B. Then, the reaction rate is interpreted as the degree of confidence that we have $A \& B$.

Similarly here, we can interpret the values a_i as degree of confidence. The function assigning a degree of confidence to each i is known as a *membership function*, or, alternatively, a *fuzzy set*.

A specific property of this fuzzy set is that all the degrees add up to!1. This property is typical for probability distributions, where the sum of probabilities of different possible events always add up to 1. So, it makes sense to call these fuzzy sets fuzzy *distribution* sets; see, e.g., [1, 2, 3, 4].

Any binary operation $r : [0,1] \times [0,1] \to [0,1]$ can be naturally extended to fuzzy distribution sets by using the formula (2). In particular, a natural extension of the minimum "and"-operation $\min(a,b)$ leads to the formula (1).

9 Difference from the usual fuzzy techniques

Please note that there is an important difference between these operations and the usual fuzzy logic.

In fuzzy logic, "and"-operations like min or product are usually associative. This makes sense, since $(A \& B) \& C$ and $A \& (B \& C)$ means the same thing.

However, in fast chemical reaction, the situation is different. Here, different ways of implementing the reaction $A+B+C \to D$ can lead to different results:

- we can first have $A+B \to AB$ and then $AB+C \to D$;
- or we can first have $A+C \to AC$ and then $AC+B \to D$;
- or we can first have $B+C \to BC$ and then $BC+A \to D$.

Sometimes, after reaction $A+B \to AB$, concentrations of AB becomes small. This happens when for each i, either $a_i \ll b_i$ or $b_i \ll a_i$. In this case, we shrink the surface for AB-molecules to speed up reactions. Depending on the order of reactions, we get different rates.

10 How to find the best order, and what next

For biological reactions, the order is pre-determined by the optimizing evolution. In contrast, in chemical engineering, we need to decide ourselves. This order optimization is a new task, not usually present in usual chemical engineering.

In general, we hope that this interpretation will help analyze complex systems of chemical reactions in biology. It may also help in chemical engineering, if we can save resources by performing several useful chemical reactions at the same time.

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