



What Principle Governs the Chemical Dynamic/Kinetic Process?

Wei-Xing Xu^{1*}

¹Newtech Monitoring Inc. 1872 Birchview Dr, Oshawa, Ontario, L1K 3B9, Canada.

Author's contribution

The sole author designed, analysed, interpreted and prepared the manuscript.

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ABSTRACT

In this work uncovered is the basic principle governing the chemical reaction dynamic/kinetic process of chemical reaction ($kt=4.6$ and $Ea/RT=4.6$), which is ignored before. Based on the "yin and yang" philosophy (see appendix A), the discovered principle has been elucidated clearly. In addition, we also demonstrate: 1. how to optimize the condition of chemical reaction, such as reaction time and temperature; 2. how to suppress the side chemical reaction. Furthermore the potential application of the discovered principle has been discussed.

Keywords: Chemical dynamic/kinetic process; ``yin and yang`` philosophy; side chemical reaction; chemical reaction condition optimization.

1. INTRODUCTION

Since the human being appeared on the earth, they found everything around them keeping change. It is the human being's character and moral that tries their best to understand the constantly changing of universe. The human being hopes to find why and how these changes

are proceeding in our universe. From the entire history of the human being, we can divide the effort of human being in understanding our universe into three stages.

First stage, due to the underdeveloped technology and observation method, the knowledge of the human being regarding our

*Corresponding author: E-mail: xweixing@hotmail.com;

universe is very finite. However, this shortcoming doesn't prohibit the human being's speculation about our universe. At this stage, the major achievements of the human being in understanding and addressing the variation about our universe are recorded in each nation's historical books or as legends in the literatures. For example, the ancient Chinese figured out "Chang'e" [1], a beautiful girl, flew to the moon and landed on it; some ancient thinkers proposed "yin and yang" philosophy [2] to explain the phenomenon observed by the human being. The detail regarding "yin and yang" philosophy is put in the appendix for those who are interested to read [see appendix A].

Second stage, the human being enters the time of knowledge explosion. During this period, a series of famous scientists appeared, such as Newton [3], Einstein [4], Planck [5], Huygens [6] and Maxwell [7]. A lot of laws or principles regarding the variation of our universe have been discovered. But here we would like mentioning Arrhenius [8] and Boltzman [9], both of them paid much attention onto the dynamic/kinetic process. Especially, since the chemistry becomes independent branch of science, their theories play fundamental role in describing dynamics/kinetics of chemical reaction. Based on the theories of Arrhenius and Boltzman, the dynamic/kinetic equations of chemical reaction have been setup.

Nowadays most of chemical factories are designed and built based on the current understanding of the dynamics/kinetics of chemical reaction. Furthermore, in order to elucidate the mechanism of chemical reaction at the molecular level, the molecular beam technique has been invented [10] and successfully applied in exploring the molecular mechanism of the chemical reaction. Based on the molecular beam technique, the mechanism of chemical reaction has been revealed and elucidated at the molecular level.

Now, most of people believe that the theory of chemical reaction has been setup, and basic principle of chemical reaction has been clearly understood and only thing left is to find or design new chemical reaction. Scientist only needs to elucidate the mechanism of chemical reaction and setup the dynamic/kinetic equation of chemical reaction from the current knowledge regarding the mechanism of chemical reaction. Nobody doubts that the understanding the chemical reaction and revealing the mechanism

of chemical reaction is even if not finished, at least nearly finished.

However, after reviewing the whole history of the research achievement in the field of the dynamics/kinetics of chemical reaction, we find the exploring the dynamics/kinetics of chemical reaction is far from finished yet. For example, most of people believe that the molecular beam technique offers us a tool to reveal the mechanism of chemical reaction at the molecular level, but just as we pointed out in the previous work [11], when using the molecular beam technique to explain the mechanism of chemical reaction, the optical effect induced by the collision between/among the reactant molecules is usually ignored, which may lead to misinterpreting the mechanism of chemical reaction.

Now the century enters 21st, the situation will change, which we may define as third stage. In this work, we will re-explore the mechanism of chemical reaction based on "yin and yang" philosophy developed in the ancient time of China. Even though we mainly discuss the dynamics/kinetics of chemical reaction, the conclusion drawn in this work can be applied onto all dynamic/kinetic processes in our universe.

2. THEORY AND DISCUSSION

Here we start our topics from the first order kinetic equation of chemical reaction [12]:

$$\frac{d(C_0 - C)}{dt} = kC \quad (1)$$

Where C_0 , C , t and k are starting concentration of reactant, concentration of reactant at time t , the reaction time and the rate constant of chemical reaction, respectively.

$$-\frac{dC}{dt} = kC \quad (2)$$

$$-\frac{dC}{C} = kdt \quad (3)$$

$$\int_{C_0}^C \frac{dC}{C} = -\int_0^t kdt \quad (4)$$

$$\ln \frac{C}{C_0} = -kt \quad (5)$$

$$C = C_0 e^{-kt} \quad (6)$$

Most of people may think the equations from (1) to (6) have completely revealed the kinetics of

chemical reaction. However, the “yin and yang” philosophy told us everything in our universe consists of “yin” and “yang” perspectives. It looks from equation (1) to equation (6) have nothing to do with “yin” and “yang” characters. In following, we start demonstrating how to reveal this missing knowledge in understanding the mechanism of chemical reaction.

Based on the mathematical principle (see appendix B), the equation (6) can be rewritten as,

$$C = C_0(1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} + \dots) \quad (7)$$

where $x=kt$.

From the terms in the bracket (see equation (7)), we know that the positive terms make the reactant concentration increase, whereas the negative terms make the reactant concentration decrease. This fact tells us that even as simple as the first order kinetic process, the chemical reaction is still governed by the positive reaction and reverse reaction (for convenience of discussion, hereafter we define from A----->B as positive reaction, from B----->A as reverse reaction and A, B are reactant and product, respectively). Here we can call the positive reaction (r_+) as “yang” and the reverse reaction (r_-) as “yin”, which can be expressed as,

$$r_+ = -x - \frac{x^3}{3!} - \frac{x^5}{5!} - \dots \quad (8)$$

$$r_- = \frac{x^2}{2!} + \frac{x^4}{4!} + \frac{x^6}{6!} + \dots \quad (9)$$

Then equation (6) can be written as,

$$C = C_0(1 + r_+ + r_-) \quad (10)$$

Based on the mathematical principle (see appendix B), we can get,

$$r_+ + r_- + 1 = e^{-x} \quad (11)$$

$$r_- - r_+ + 1 = e^x \quad (12)$$

$$r_+ = \frac{e^{-x} - e^x}{2} \quad (14)$$

$$r_- = \frac{e^{-x} + e^x}{2} - 1 \quad (15)$$

2.1 How to Determine the Best Chemical Reaction Time?

In order to make the chemical reaction proceeds in positive direction efficiently, we have to make

$|r_+| - |r_-|$ reaches the maximum. Fig.1 shows the relation between x and $\Delta r (= |r_+| - |r_-|)$. From Fig.1, we know that as long as $x \approx 4.6$, the $\Delta r (= |r_+| - |r_-|)$ reaches the maximum. Here x is a dimensionless parameter which does not depend on other factors. Therefore, it is a universal constant for all the first order dynamic/kinetic processes. From this constant, we can determine when the chemical reaction will reach the maximum. Based on the relation, $x=kt$, (where $x=4.6$), the optimized reaction time can be determined.

Another important meaning of the relation, $x=kt$, is that if the chemical reaction exists side reaction, (see Fig.2), we can determine when the side reaction will reach the maximum. This result offers us an alternative way to design or select the chemical reaction route to greatly avoid or suppress the side reaction.

2.2 How to Determine the Best Chemical Reaction Temperature

From the current dynamic/kinetic theory of the chemical reaction, we know that,

$$k = Ae^{-\frac{E_a}{RT}} \quad (16)$$

where k , A , E_a , R and T are the rate constant of chemical reaction, pre-exponential factor of the chemical reaction rate, activation energy, Gas constant and temperature, respectively.

Following the similar discussion above (see 2.1 paragraph), in order to make the chemical reaction proceeds in positive direction efficiently,

$$\frac{E_a}{RT} = 4.6 \quad , \text{ then } T = \frac{E_a}{4.6R} \quad (17)$$

This relation offers us a way to select the best chemical reaction temperature and at the optimized temperature, the positive chemical reaction will reach the maximum.

2.3 How to Determine the Positive and Reverse Chemical Reaction Activation Energy

Traditionally, we determine the equilibrium constant of chemical reaction [13] by

$$K = \frac{k_+}{k_-} \quad (18)$$

Where K is equilibrium constant, k_+ and k_- are the rate constant of positive chemical reaction and

the rate constant of reverse chemical reaction, respectively. Here we offer a different way to determine the activation energy of chemical reaction as long as we can determine one of them, that is, the activation energy of positive chemical reaction or the activation energy of reverse chemical reaction. Now we demonstrate how to do on the discussion above.

In equilibrium,

$$r_+ = r_- \quad (19)$$

$$r_+ = \frac{e^{-x}-e^x}{2}, \text{ where } x = \frac{E_a}{RT} \quad (20)$$

$$r_- = \frac{e^{-(x+\Delta x)}+e^{(x+\Delta x)}}{2} - 1 \quad (21)$$

Under the equilibrium requirement,

$$\frac{e^{-x}-e^x}{2} = \frac{e^{-(x+\Delta x)}+e^{(x+\Delta x)}}{2} - 1 \quad (22)$$

By rearrangement, we get,

$$e^x \times e^{2\Delta x} + (e^x - e^{-x} - 2)e^{\Delta x} + e^{-x} = 0 \quad (23)$$

$$e^{\Delta x} = \frac{(2+e^{-x}-e^x) \pm \sqrt{(2+e^{-x}-e^x)^2-4}}{2e^x} \quad (24)$$

$$\Delta x = \ln \left[\frac{(2+e^{-x}-e^x) \pm \sqrt{(2+e^{-x}-e^x)^2-4}}{2e^x} \right] \quad (25)$$

Therefore, the activation energy of reverse chemical reaction can be determined, that is,

$$E_b = E_a + RT \ln \left[\frac{(2+e^{-x}-e^x) \pm \sqrt{(2+e^{-x}-e^x)^2-4}}{2e^x} \right] \quad (26)$$

where $x = \frac{E_a}{RT}$, and E_b is the activation energy of reverse chemical reaction.

Based on the equation (26), we can determine the activation energy of reverse chemical reaction through the activation energy of positive reaction and vice versa. The activation energy of positive chemical reaction and the activation energy of reverse chemical reaction are related by equation (26), not independent each other.

From the discussion above, we know that the dynamic/kinetic processes do have “yin” and “yang” perspectives. This “yin” and “yang” perspectives are competitors in the dynamic/kinetic process. “yin” and “yang” are not independent but related each other, just as “yin and yang” philosophy’s explanation regarding everything in our universe. Therefore, “yin and yang” philosophy is generally valid principle to explain the phenomenon in our universe.

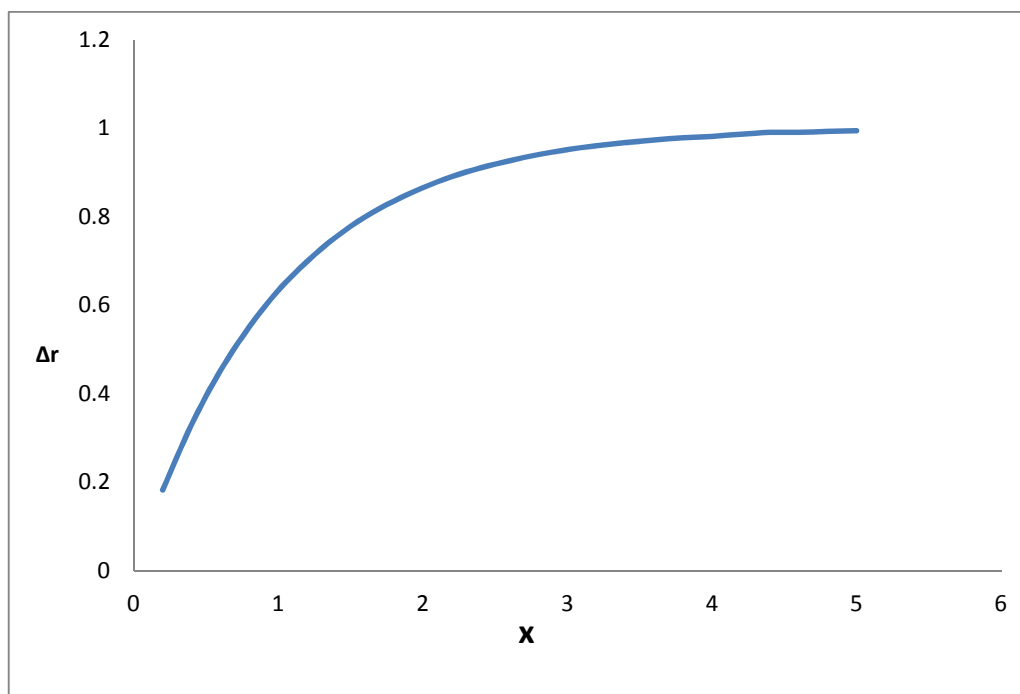


Fig.1 The Relation between $\Delta r(=|r_+| - |r_-|)$ and $X(=kt)$

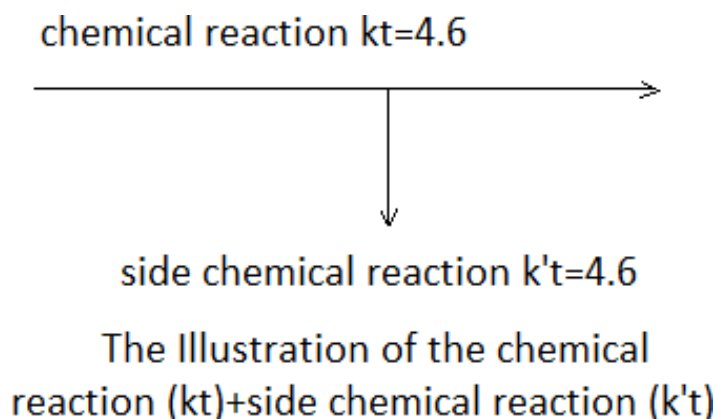


Fig. 2. The illustration of the chemical reaction (kt) +side chemical reaction $(k't)$

The understanding of the chemical reaction, based on the “yin” and “yang” principle, makes us clear all the dynamic/kinetic processes are going on in the alternative way under “yin” and “yang” principle, including the chemical reaction. That is the reason why the chemical reaction proceeds in a way like a wave, only difference among the chemical reactions is just in that some of chemical reactions show the wave-like behaviour more obvious, some are less obvious.

Now we understand why the constant (4.6) frequently appears in the dynamic/kinetic processes and this constant (4.6) should be generally valid in the nature which governs the dynamic/kinetic processes in our universe.

3. POTENTIAL APPLICATION

Here we would spend some time to discuss the potential application regarding the principle discovered in this work.

3.1 How to Select the Best Chemical Reaction Route

As we discussed in this work, the constant (4.6) frequently shows up in the process of chemical reaction. From the constant (4.6), we can determine when and what temperature the chemical reaction will reach the maximum, and the most important, it shows us when and what temperature the side chemical reaction will obviously occur. Therefore, we can optimize the chemical reaction time and temperature to avoid or suppress the side product in the chemical reaction process. This discovery may cause the revolution in designing and building the chemical factory.

3.2 How the Discovery in This Work Influences on the Other Dynamic and Kinetic Processes?

As we discussed above, the constant (4.6) is generally valid in all dynamic/kinetic processes. Therefore, all dynamic/kinetic systems can be analyzed in the same way above, such as the diffusion process, current transportation in conductor and heat dissipation process.

3.3 What's Meaning of the Discovery in this Work For the Biology System?

To our knowledge, the biology system contains a lot of chemical reactions. Here we would like taking the human body as an example. As we discussed in this work, the chemical reaction consists of two perspectives, that is, “yin” and “yang”. Therefore, the “yin” and “yang” of all chemical reactions going on in the human body takes effect in cooperative way. All “yin” and “yang” of the chemical reaction forms total circulation system in the human body. This kind of circulation called “Qi” from the “yin” and “yang” philosophy. This “Qi” circulation in the human body forms the circulation network. This kind of “Qi” circulation has been described by the “yin and yang” philosophy. After certain time development, the ancient Chinese found the nodes in the circulation network. This kind of nodes in the circulation system is found and named as acupuncture point. Following the circulation system, the ancient Chinese can treat the disease of people and keep the people in health condition. These kinds of knowledge help Chinese setup the medical system called Chinese traditional medicine and acupuncture technology.

Here we would like pointing out that the circulation systems are formed by a series of chemical reactions going on in the human body. We can speculate that the relation between dynamic/kinetic constants and time discovered in this work are valid, then we can determine the lifetime of the human being by

$$\sum_{i=1}^n k_i t = 4.6 \times n \quad (27)$$

where n is total number of chemical reactions proceeding in the human body, k_i is each constant of chemical reaction, then,

$$t = \frac{4.6 \times n}{\sum_{i=1}^n k_i} \quad (28)$$

If we can determine each k_i , then t is the lifetime of the human being.

4. CONCLUSION

In this work the principle governing the dynamic/kinetic process of chemical reaction has been revealed. The ``yin and yang`` philosophy elucidates the discovered principle clearly. Just as we discussed in this work, the discovery in this work will find wide application in designing chemical factory, selecting the chemical reaction route, suppressing the side reaction and many dynamic/kinetic processes, which may lead to the revolution in these fields.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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APPENDIX A

“yin and yang” can be thought of as complementary (rather than opposing) forces that interact to form a dynamic system in which the whole is greater than the assembled parts. According to this philosophy, everything has both “yin and yang” aspects which push the system constantly evolving. Therefore, the ancient Chinese thinker believed that “yin and yang” principle is generally valid in our universe.

APPENDIX B

From the literature, we know that,

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots \quad (b1)$$

$$e^{-x} = 1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} + \dots \quad (b2)$$

Here we can define two series, that is,

$$S_1(x) = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \frac{x^6}{6!} + \dots \quad (b3)$$

$$S_2(x) = -x - \frac{x^3}{3!} - \frac{x^5}{5!} - \dots \quad (b4)$$

Then,

$$S_1(x) - S_2(x) = e^x \quad (b5)$$

$$S_1(x) + S_2(x) = e^{-x} \quad (b6)$$

From equation (b5) and equation (b6), we can get,

$$S_1(x) = \frac{e^x + e^{-x}}{2} \quad (b7)$$

$$S_2(x) = \frac{e^{-x} - e^x}{2} \quad (b8)$$

The function $S_1(x)$ and $S_2(x)$ have following properties,

$$S_1^2(x) + S_2^2(x) = \frac{(e^{2x} + e^{-2x})}{2} \quad (b9)$$

$$S_1^2(x) - S_2^2(x) = 1 \quad (b10)$$

$$S_1(x) \times S_2(x) = \frac{(e^{-2x} - e^{2x})}{4} \quad (b11)$$

$$S_1'(x) = -S_2(x) \quad (b12)$$

$$S_2'(x) = -S_1(x) \tag{b13}$$

$$S_1''(x) = S_1(x) \tag{b14}$$

$$S_2''(x) = S_2(x) \tag{b15}$$

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