

## Application of Higher Mathematics in Different Disciplines - Taking Chemical Thermodynamics as an Example

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As a basic subject, higher mathematics has been widely applied in various disciplines and all aspects of life. This article, based on higher mathematics thoughts, introduces basic concepts of higher mathematics such as calculus to analyze the application of higher mathematics in chemical thermodynamics. In this paper, the continuity and total differential properties of chemical thermodynamic state functions are summarized, and the derivation of thermodynamic formula is accomplished through these properties and the principle of calculus. This paper discusses the relation and difference between the process function and the state function to avoid the confusion of concepts in the process of thermodynamics calculation. It also points out the significance of higher mathematics in studying thermodynamics and the necessary of using higher mathematics to solve and deal with chemical problems. The application of higher mathematics can provide a better understanding on chemical thermodynamics and cultivate the ability to solve practical problems with higher mathematics knowledge and thoughts.

### 1. Introduction

With the rapid development of social science and technology and economy, the demand and cultivation of talents is the source and motive force to maintain social development. In the era of knowledge economy, people attach more importance to science education and students' comprehensive scientific literacy (Etzkowitz and Leydesdorff, 1997; Cooke, 2001; Leu, 2005; Chen, 2002). Higher mathematics is a basic discipline that can promote students' comprehensive scientific literacy. With the development of interdisciplinary, the application of higher mathematics is more and more wide covering all aspects of daily life from basic subjects such as chemistry, physics, and medicine to applied disciplines such as economic management (Gray et al., 1999; Weber, 2004; Harriss, 2002). Higher mathematics not only is a basic subject, but also contains mathematics thoughts with an important significance in viewing, analyzing and solving problems, as well as making a choice (Laugksch, 2000; Shamos and Howes, 1996).

Chemistry is a subject to study the existence and transformation of substances (Gierer, 1982). At first, chemical knowledge is accumulated through a large number of experiments. With the development and research of the discipline, chemists realize the important role of higher mathematics in studying chemical theories, which has brought a breakthrough. They start to describe and simplify chemical problems by mathematical abstract language and tools, as well as change from qualitative analysis to quantitative calculation, from experimental results to theoretical formula derivation (Schreiber, 2002). For chemical thermodynamics, this paper introduces basic concepts of higher mathematics such as calculus to analyze the application of higher mathematics in chemical thermodynamics with examples and uses mathematics thoughts to solve and deal with chemical problems, providing a better understanding of chemical thermodynamics and cultivating the ability to solve practical problems with higher mathematics knowledge and thoughts (Dehaene et al., 1999; Duval, 1999).

## 2. Application of higher mathematics

### 2.1 Higher mathematics

As public basic course of colleges and universities, higher mathematics is mainly composed of six parts: differential calculus, integral calculus and analytic geometry, differential equation, series theory and limit theory. The relationship among them is shown in Figure 1.

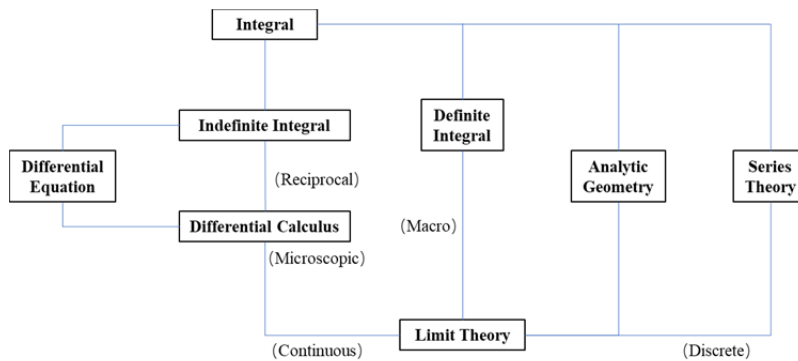


Figure 1: Framework of advanced mathematics

### 2.2 Higher mathematics thoughts

Mathematics thoughts are the exploration and understanding of the essence of mathematical knowledge and methods. In the learning of higher mathematics, on the one hand, concrete knowledge is learned to form the "skeleton" (Tall et al., 2005). On the other hand, the cultivation of mathematics thoughts is more important as the "soul". Knowledge is connected to form an organic whole with a deep understanding about mathematics thoughts. Therefore, the mastery of higher mathematics thoughts is the key to learning, and the motivation for acquiring knowledge, developing logical thinking ability, migration ability and re-creation ability (Borba and Villarreal, 2005; Bybee, 1997). The following Figure 2 shows the significance of strengthening the cultivation and teaching of higher mathematics thoughts.

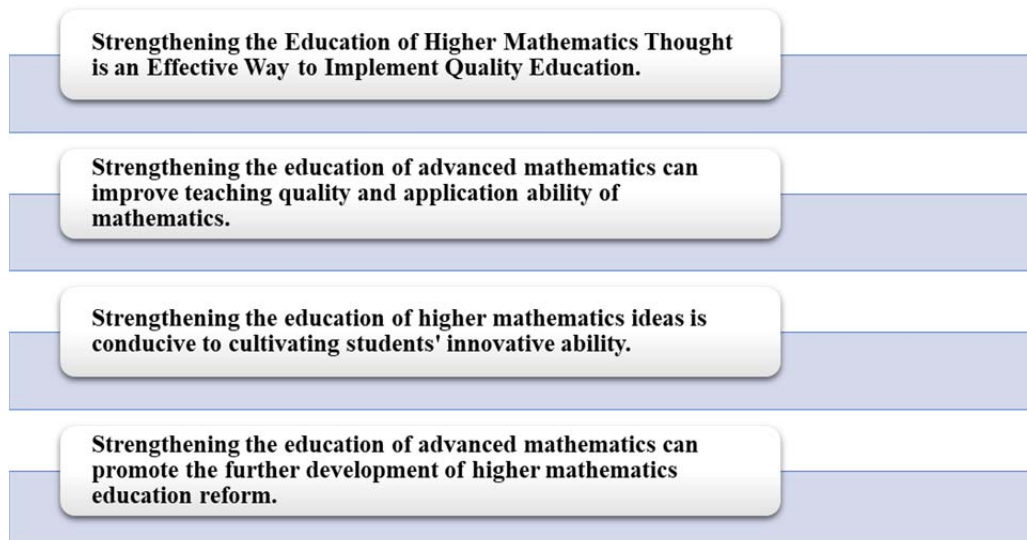


Figure 2: Significance of cultivating advanced mathematics thoughts

### 2.3 Application of higher mathematics

Higher mathematics has penetrated every aspect of our life and work as shown in Figure 3 from intelligent robots, personal investment ways to goods illustrations, various reports and charts. Higher mathematics knowledge and literacy are needed to observe, analyze, and make a choice and decision.

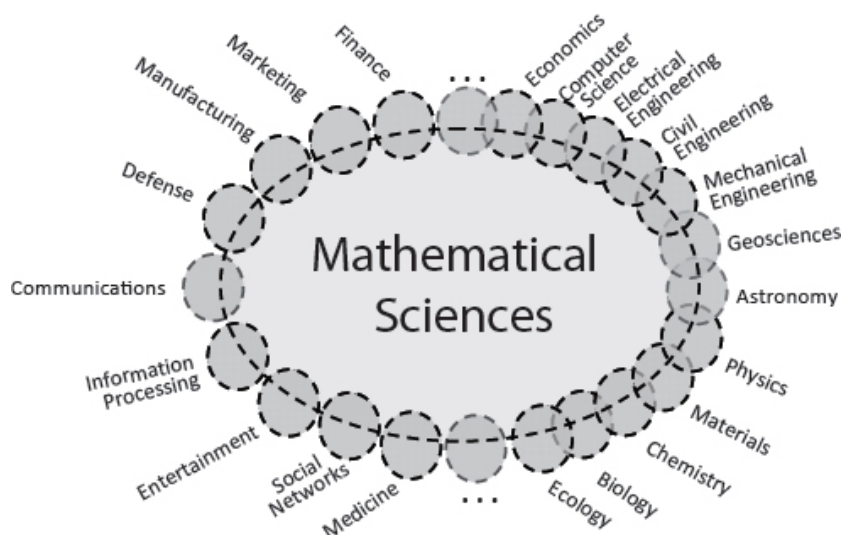


Figure 3: Scope of application of advanced mathematics

### 3. Introduction of higher mathematics in chemical thermodynamics

#### 3.1 Significance of introducing higher mathematics in chemical thermodynamics

Chemistry's early development mainly relies on the experience and results of experiments. Many chemists think that the introduction of higher mathematics makes problems more complicated due to the unclear cognition of mathematics theories and thoughts. However, as the accumulation of knowledge and the systematic construction of theoretical knowledge, chemists begin to seek abstract mathematical tools to solve chemical problems and clarify the importance of introducing higher mathematics through constant practices. It has been proved that experiments and theories are both essential for physics and chemistry. With the characteristics of strong logicity, various formulas and abstract theories, it is of great significance to use higher mathematics as a tool for promoting the theory development and innovation and solving practical problems.

#### 3.2 Application fundamentals of higher mathematics in chemical thermodynamics

In a classical study of thermodynamics, it is assumed that substances are continuum without considering the their microstructure. Therefore, thermodynamic state functions can be used. The change of thermodynamic functions is continuous in a certain range. According to this assumption, calculus can be introduced into chemical thermodynamic functions, because the premise of calculus is that the function is continuous.

In chemical thermodynamics, quantities that are independent of the process are called "state functions", and their characteristics can be expressed and described in mathematical language. Basic state functions are shown in Figure 4 including  $p$ ,  $V$ ,  $T$ ,  $U$  and  $S$ .

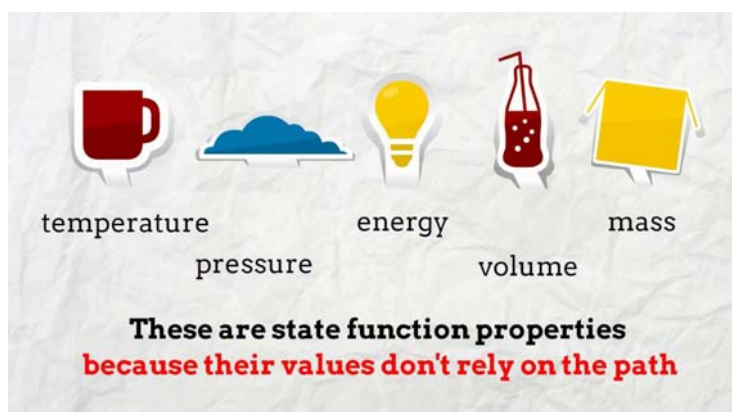


Figure 4: Basic state functions

Three features of state functions and corresponding mathematical language are shown in Figure 5.

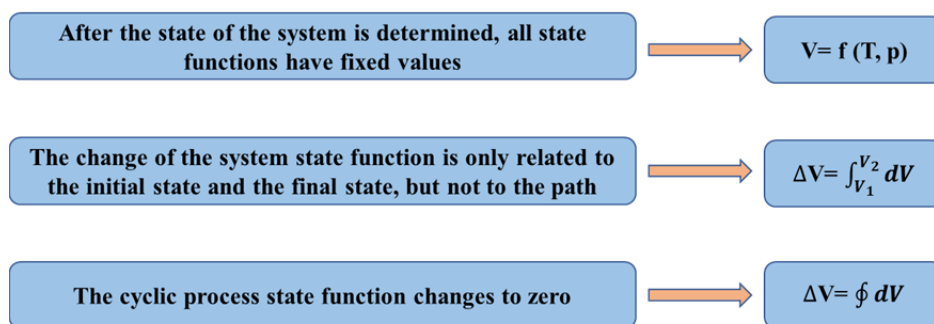


Figure 5: Features of state functions

## 4. Application of higher mathematics in chemical thermodynamics

### 4.1 Formula derivation through higher mathematics

There are too many formulas in the chemical thermodynamics, so it is difficult to remember all of them. But the derivation and application are closely related to higher mathematics. People who master higher mathematics knowledge can easily understand and make use of the nature and characteristics of formulas to derive, rather than learning by rote with more mistakes.

#### 4.1.1 Derivation of maxwell relations

Maxwell relations are an important set of equations in thermodynamics. It is an alternative equation to convert thermodynamic state functions that are difficult to measure into that are easy to measure. Only the total differential property of state functions is used in this derivation.

For any state functions  $z=f(x,y)$ , the total differential can be obtained:

$$dz = \left(\frac{\partial z}{\partial x}\right)_y dx + \left(\frac{\partial z}{\partial y}\right)_x dy$$

Because the second order partial derivative of the total differential is not related to the order, it obtains:

$$\left[\frac{\partial}{\partial y}\left(\frac{\partial z}{\partial x}\right)_y\right]_x = \left[\frac{\partial}{\partial x}\left(\frac{\partial z}{\partial y}\right)_x\right]_y$$

Then, according to the basic equation of thermodynamics,  $dU=TdS-pdV$ , Maxwell relations are deduced as follows:

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V, \left(\frac{\partial T}{\partial p}\right)_S = -\left(\frac{\partial V}{\partial S}\right)_p, \left(\frac{\partial p}{\partial T}\right)_V = -\left(\frac{\partial S}{\partial V}\right)_T, -\left(\frac{\partial V}{\partial T}\right)_p = -\left(\frac{\partial S}{\partial p}\right)_T, \text{ where } p, V, T, \text{ and } S \text{ represent pressure, volume, temperature and entropy, respectively.}$$

#### 4.1.2 Derivation of corresponding coefficient relations

Corresponding coefficient relations in chemical thermodynamics reveals the universality of all systems and is the basis of thermodynamics. According to the fundamental equation of thermodynamics,  $dU=TdS-pdV$ , the total differential form of the thermodynamic function can be obtained by the total differential property of state functions:

$$dU = \left(\frac{\partial U}{\partial S}\right)_V dS + \left(\frac{\partial U}{\partial V}\right)_S dV$$

According to equal corresponding terms, the corresponding coefficient relations can be deduced:

$$\left(\frac{\partial U}{\partial S}\right)_V = T, \left(\frac{\partial U}{\partial V}\right)_S = -p, \left(\frac{\partial H}{\partial S}\right)_p = T, \left(\frac{\partial H}{\partial p}\right)_S = V, \left(\frac{\partial G}{\partial T}\right)_p = -S, \left(\frac{\partial G}{\partial p}\right)_T = V, \left(\frac{\partial A}{\partial T}\right)_V = -S, \left(\frac{\partial A}{\partial V}\right)_T = -p, \text{ where } p, V, \text{ and } T \text{ represent pressure, volume and temperature, respectively, as well as } U, H, A, G, \text{ and } S \text{ respectively represent internal energy, enthalpy, Helmholtz free energy, Gibbs free energy and entropy.}$$

## 4.2 Application of higher mathematics in understanding chemical thermodynamics

### 4.2.1 State functions and process variables

State functions and process functions are two kinds of important physical quantities that are easy to be confused in thermodynamics. Table 1 shows the comparison of state functions and process functions from the

aspect of physics and mathematics. After the mathematical analysis, the difference between them is more obvious.

Table 1: The comparison of state function and process function

	State Function	Process Variable
<b>Physical</b>	The state function belongs to the nature of matter and is a representation of the state of the system.	Process variables are characterizations of processes that arise during system changes and cannot exist independently of processes.
<b>Mathematical</b>	$U=(S,V)$ There is Full differential	$\delta Q = CdT$ There is no full differential

The difference between  $dU$  and  $\Delta U$  is analyzed from the angle of mathematics. Although both of them represent a difference,  $dU$ , a very small uncertain difference, is the infinitesimal and the differential of  $U$ , which can be used for the integral. However,  $\Delta U$  represents a definite difference, as the result of the integral. Therefore, both  $dU$  and  $\Delta U$  are mathematically different.

#### 4.2.2 Reversible and non-reversible processes

Thermodynamics is based on the equilibrium state. Only the equilibrium system can be expressed by the state function of thermodynamics. For the reversible process, every change is in equilibrium. Thus, you can use calculus, such as the following formula for the reversible volume work.

For reversible expansion or compression:

$$P_E = p \pm dp, \delta W = -P_E dV$$

For this process, the integral is:

$$W = - \int_{V_1}^{V_2} P_E dV = - \int_{V_1}^{V_2} (p \pm dp) dV = - \int_{V_1}^{V_2} p dV \pm \int_{V_1}^{V_2} dp dV$$

The formula for reversible volume work can be obtained by omitting the second order infinitesimal:

$$W = - \int_{V_1}^{V_2} p dV$$

For the non-reversible process, the non-reversible process must be converted into an equivalent reversible process.

#### 4.3 Physical quantities and related calculation

With the help of higher mathematical language, the expression of thermodynamical concepts can be more concise. The expression of the relationship and transformation among physical quantities are also more intuitive and precise.

##### 4.3.1 Definition of heat capacity

Without phase and chemical changes, heat exchanges of systems and environment and the resulting temperature changes are called heat capacity, which is expressed in higher mathematical language C:

$$C = \frac{\delta Q}{dT}$$

In the calculation of thermodynamics, there are two commonly used concepts including constant volume heat capacity  $C_{V,m}$  and isobaric heat capacity  $C_{p,m}$ .

For the constant volume process of non-volume work:

$$\delta Q_V = dU, C_{V,m} = \frac{1}{n} \frac{\delta Q_V}{dT} = \left( \frac{\partial U_m}{\partial T} \right)_V$$

For the constant pressure process of non-volume work:

$$\delta Q_p = dH, C_{p,m} = \frac{1}{n} \frac{\delta Q_p}{dT} = \left( \frac{\partial H_m}{\partial T} \right)_p$$

##### 4.3.2 Relationship between $C_{V,m}$ and $C_{p,m}$

$$C_{p,m} - C_{V,m} = \left( \frac{\partial H_m}{\partial T} \right)_p - \left( \frac{\partial U_m}{\partial T} \right)_V = \left( \frac{\partial (U_m + pV_m)}{\partial T} \right)_p - \left( \frac{\partial U_m}{\partial T} \right)_V = \left( \frac{\partial U_m}{\partial T} \right)_p + p \left( \frac{\partial V_m}{\partial T} \right)_p - \left( \frac{\partial U_m}{\partial T} \right)_V$$

For 1 mol pure substance:  $U_m = f(T, V)$

$$dU_m = \left( \frac{\partial U_m}{\partial T} \right)_V dT + \left( \frac{\partial U_m}{\partial V_m} \right)_T dV_m, \left( \frac{\partial U_m}{\partial T} \right)_p = \left( \frac{\partial U_m}{\partial T} \right)_V + \left( \frac{\partial U_m}{\partial V_m} \right)_T \left( \frac{\partial V_m}{\partial T} \right)_p, C_{p,m} - C_{V,m} = \left( \frac{\partial U_m}{\partial T} \right)_p + p \left( \frac{\partial V_m}{\partial T} \right)_p - \left( \frac{\partial U_m}{\partial T} \right)_V,$$

$$C_{p,m} - C_{V,m} = \left( \frac{\partial U_m}{\partial T} \right)_V + \left( \frac{\partial U_m}{\partial V_m} \right)_T \left( \frac{\partial V_m}{\partial T} \right)_p + p \left( \frac{\partial V_m}{\partial T} \right)_p - \left( \frac{\partial U_m}{\partial T} \right)_V, C_{p,m} - C_{V,m} = \left( \frac{\partial V_m}{\partial T} \right)_p \left[ \left( \frac{\partial U_m}{\partial V_m} \right)_T + p \right]$$

For ideal gas,  $U = f(T) \left( \frac{\partial U_m}{\partial V_m} \right)_T = 0$

$$\text{Thus, } C_{p,m} - C_{v,m} = p \left( \frac{\partial V_m}{\partial T} \right)_p = p \left( \frac{\partial \left( \frac{RT}{p} \right)}{\partial T} \right)_p = p \cdot \frac{R}{p} = R$$

$C_{p,m} - C_{v,m} = R$ , where  $R$  is the general gas constant, and its value is related to the unit rather than the type of gas.

## 5. Conclusion

This paper introduces basic concepts of higher mathematics, such as calculus, into chemical thermodynamics to analyze the application of higher mathematics in chemical thermodynamics. Specific research results are as follows:

- (1) to introduce the significance and basis of introducing higher mathematics into chemical thermodynamics, namely, the thermodynamic function is continuous and can be expressed in calculus;
- (2) to compare state functions and process functions from perspectives of mathematics and physics, so as to avoid confusion in the use of thermodynamical concepts;
- (3) to combine the concept of calculus, mathematics thoughts and theories of chemical thermodynamics. This paper introduces the continuity, abstract and total differential properties of thermodynamics functions to complete the thermodynamics formula derivation and improve the understanding of concepts.

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