

Designing a Learning Project on Thermodynamics for Chemistry Students According to the CDIO Teaching Mode

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Abstract General chemistry programs at universities around the world often focus on learning from the first and second school year, in which knowledge of thermodynamics plays a fundamental role in studying the theory of chemical processes. Although it is learned early at universities that train chemistry students, but with the content is difficult and complex when developing the application of thermodynamic principles to chemical processes occurring in closed systems to research chemical equilibrium, has caused many students to lose their learning direction, leading to not good academic results. In order to overcome those difficulties, we designed a learning project based on the CDIO teaching mode to guide students in forming project ideas, project design, project implementation and operation. Through the project, students will easily access thermodynamic issues to evaluate a chemical process occurring, creating a strong motivation for students to research chemistry.

Keywords: CDIO teaching mode, learning project, project based teaching, chemistry, thermodynamics

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1. Introduction

The CDIO teaching mode emphasizes basic principles, placed in the context of Ideation - Design - Implementation - Operation, bringing many practical benefits [1]: The curriculum is organized around courses that support each other but have closely interwoven CDIO activities; Rich with student design-build-test projects; Integrate learning of professional skills such as teamwork and communication; Active and experiential learning features.

Project teaching based on the CDIO approach will be an ideal model for students to easily learn complex and difficult knowledge such as thermodynamics problems for chemistry students at universities. To design a learning project according to the CDIO approach, students can follow the diagram depicted in Figure 1. The application process is as follows:

Task conception and decomposition: Analyze the context, identify problems and form ideas for the project.

Project design: Overview of research documents related to the project. Analyze documents and propose specific measures for project implementation.

Project implementation: Implement the project based on proposed measures, find solutions to research problems.

Project sumary and evaluation: Operate the project for a specific problem, summarize and evaluate the advantages and limitations (if any) of the project.



Figure 1. Project teaching based on the CDIO teaching mode

2. Content and Research Methods

2.1. Task Conception and Decomposition

Thermodynamics is fundamental and difficult knowledge for chemistry students when studying General Chemistry. However, among the many knowledge contents of thermodynamics, we see that only 3 state functions, namely enthalpy (H), entropy (S) and Gibbs function (G) are the most important because they can answer questions that each student always poses to themselves is a challenge that needs to be conquered when studying chemistry. Questions that students often ask when studying thermodynamics:

(1) Why can this reaction occur while the other reaction cannot occur?

(2) Why can this reaction occur under normal conditions but the other reaction can only occur at a specific temperature (T)?

(3) How do we need to adjust temperature, concentration, pressure or catalyst so that the reversible reaction occurs in the most favorable direction?

(4) How to build a mathematical expression to clarify Le Chatelier's equilibrium shifting principle?

Instructors can pose a question for students to propose ideas for learning projects: Among the four factors including pressure, temperature, concentration and catalyst, which factor influenced the change of the above 3 state functions?

From the set of 4 questions above, students realize that the temperature factor changes the values of the 3 state functions. Through that analysis, students will form a learning project with a hypothetical name: *Research the influence of temperature on the change in the value of the three state functions enthalpy, entropy and Gibbs free energy function.*

2.2. Project Design

Before designing the project, students must search for documents related to the project idea. This is an important step for students to overview the core issues of the topic.

Research by Hafid Sokrat and colleagues [2] shows that the nature of the concepts of enthalpy, entropy and Gibbs free energy is very difficult because first-year students are not equipped with adequate mathematical knowledge to study chemistry. In particular, this difficulty is not only encountered in Vietnamese students but also in international students, affecting the psychology of students' laziness in learning chemistry.

History of invention of state functions: In 1840, Hess invented the enthalpy function; In 1824, Carnot invented the entropy function; In 1870, Gibbs was the first to introduce the concept of free energy that bears his name [3]. Many studies on thermodynamics show that the methods of approaching and constructing state functions are mainly traditional and academic [4,5].

Some properties of Gibbs free energy have been specified [6,7]:

- For reversible reactions, when the Gibbs free energy

 $(\Delta_r G_T^\circ)$ has a negative value, the reaction will occur in the forward direction and when it has a positive value,

- When $\Delta_{\rm r} G_{\rm T}^{\rm o} = 0$ deduced

 $G^{\circ}(\text{products}) = G^{\circ}(\text{reatants})$ and at the vertex of the parabola of the graph representing the dependence of Gibbs energy on the reaction process, there will be Q = K = 1, where Q is the quotient of the product concentration (pressure) of the product compared to the reactant and K is the equilibrium constant.

- The shape of the graph represents the dependence of Gibbs energy on the probability of a reaction occurring.

- Using the Gibbs–Helmholtz equation [8] to build the liquid-gas equilibrium of CO_2 at different temperature values:

$$\frac{\Delta_{\rm r}G_{\rm T}^{\rm o}}{T} = \frac{\Delta_{\rm r}G_{298}^{\rm o}}{298} - \int_{298}^{\rm T} \frac{\Delta_{\rm r}H_{\rm T}^{\rm o}}{T^2} \, dT$$

Gibbs was the first to postulate the relationship of eight thermodynamic quantities: pressure, volume, temperature, entropy, internal energy, enthalpy, Gibbs energy and work on the same 3-dimensional space diagram to describe chemical equilibrium of a system [9].

For reactions occurring under standard conditions, calculating the enthalpy of the reaction is relatively simple, but more importantly, it helps students clearly understand the relationship of enthalpy change with the breakdown and formation of bond energy [10].

David Keifer suggested that the default expression for enthalpy in Physical Chemistry textbooks should not be $\Delta H = q_p = \Delta U + P\Delta V$ but to add a quantity ($w_{additional}$) in the enthalpy expression. That means $\Delta H = q_p + w_{additional}$ with $w_{additional}$ to be work does not expand [11].

Transforming the Gibbs-Helmholtz equation into the form: $\frac{dlnK_p}{dT} = \frac{\Delta_r H_T^o}{RT^2}$ will help students easily calculate the equilibrium constant Kp of the ammonia synthesis reaction at different temperatures [12].

Using mathematical knowledge, students will build the equation k = f(T) from the Arrhenius equation $k = Ae^{-\frac{E_a}{RT}}$ to calculate the rate constant of the reaction at different temperatures [13].

Roger Araujo established the Gibbs function according to the traditional method and calculated the equilibrium constant of the oxidation reaction of Fe^{2+} ions to Fe^{3+} under the influence of oxygen gas [14].

After studying the theory, we see that the enthalpy $(\Delta_{f}H_{298}^{o})$, entropy (S_{298}^{o}) and Gibbs free energy $(\Delta_{f}G_{298}^{o})$ values of the substance (under standard conditions) are easy to look up. So if the experiment is conducted at a temperature other than 25 °C, will these values change and what are their values?

Therefore, we need to build a general mathematical expression that shows the relationship of the values of enthalpy, entropy and Gibbs free energy according to the temperature. Mean:

$$\Delta_{f} H_{T}^{o} = \Delta_{f} H_{298}^{o} + aT + \dots$$
$$S_{T}^{o} = S_{200}^{o} + bT + \dots$$

 $\Delta_{f}G_{T}^{\circ} = \Delta_{f}G_{298}^{\circ} + cT + ...$ In other words, enthalpy, entropy and Gibbs free energy of a substance are functions that depend on temperature.

2.3. Project Implementation

With knowledge of derivatives, differentials and integration, students can build the dependence of each state function on temperature.

(1) For the enthalpy function

Derived from the expression for calculating the change in heat capacity of the reaction:

$$\Delta_{\rm r} C_{\rm p} = \frac{d\Delta_{\rm r} H}{dT}$$
(1.1)

Kirchhoff separated the variables, then integrated both sides of equation (1.1) and the temperature changed from 298 K to T, we get:

$$\Delta_{\rm r} {\rm H}_{\rm T}^{\rm o} = \Delta_{\rm r} {\rm H}_{298}^{\rm o} + \int_{298}^{\rm T} \Delta_{\rm r} {\rm C}_{\rm p} {\rm d}{\rm T}$$
(1.2)

(2) For the entropy function

According to the second law of thermodynamics, for reversible reactions (no phase change of the substances during the reaction), the temperature-dependent entropy is

$$d\Delta_{\rm r}S = \frac{d\Delta_{\rm r}H}{T} = \frac{\Delta_{\rm r}C_{\rm p}dT}{T}$$
(2.1)

Integrating both sides of equation (2.1) we get:

$$\int_{298}^{T} d\Delta_r S = \int_{298}^{T} \frac{\Delta_r C_p dT}{T}$$

or

$$\Delta_{\rm r} {\rm S}_{\rm T}^{\rm o} = \Delta_{\rm r} {\rm S}_{298}^{\rm o} + \int_{298}^{\rm T} \frac{\Delta_{\rm r} {\rm C}_{\rm p} {\rm d} {\rm T}}{{\rm T}} \tag{2.2}$$

(3) For the Gibbs function

We have three methods to represent the dependence of the Gibbs function on temperature.

Method 1. Use the Gibbs equation:

$$\Delta_{\rm r}G_{\rm T}^{\rm o} = \Delta_{\rm r}H_{\rm T}^{\rm o} - T\Delta_{\rm r}S_{\rm T}^{\rm o}$$

Method 2. Use equation:

$$\Delta_{\rm r}G_{\rm T}^{\rm o} = \Delta_{\rm r}G_{298}^{\rm o} - \int_{298}^{\rm T} \Delta_{\rm r}SdT \tag{3.1}$$

We set up the equation (3.1). We have:

 $\begin{cases} dH = dU + PdV \text{ (first law of thermodynamics)} \\ TdS \ge dH \text{ (second law of thermodynamics)} \end{cases}$

$$\longrightarrow$$
TdS \geq dU + PdV

When the reaction is reversible: TdS = dU + PdV or dU = TdS - PdV (3.2)

Adding the differential d(PV -TS) to both sides of equation (3.2), we get:

$$\underbrace{dU + d(PV - TS)}_{d(U + PV - TS)} = TdS - PdV + d(PV - TS)$$

$$\underbrace{d(U + PV - TS)}_{d(U + PV - TS)} = TdS - PdV + d(PV - TS)$$
(3.3)

Substituting G = U + PV - TS into (3.3) and then differentiating we get:

$$dG = \mathcal{T}dS - \mathcal{P}dV + \mathcal{P}dV + VdP - \mathcal{T}dS - SdT \rightarrow dG_{(3.4)}$$
$$= VdP - SdT$$

On the other hand, G is a function of two variables: G = f(T, P). Differentiating the function G we get:

$$d\mathbf{G} = \left(\frac{\partial \mathbf{G}}{\partial \mathbf{T}}\right)_{\mathbf{P}} d\mathbf{T} + \left(\frac{\partial \mathbf{G}}{\partial \mathbf{P}}\right)_{\mathbf{T}} d\mathbf{P}$$
(3.5)

Because G is a state function, dG is a total differential. Therefore from (3.4) and (3.5) we have:

$$\begin{cases} \mathbf{V} = \left(\frac{\partial \mathbf{G}}{\partial \mathbf{P}}\right)_{\mathrm{T}} \\ -\mathbf{S} = \left(\frac{\partial \mathbf{G}}{\partial \mathrm{T}}\right)_{\mathrm{P}} \text{ or } -\Delta \mathbf{S} = \left(\frac{\partial \Delta \mathbf{G}}{\partial \Delta \mathrm{T}}\right)_{\mathrm{P}} \end{cases}$$
(3.6)

Separating the variables, then integrating both sides of equation (3.6), we get the equation (3.1):

$$\int_{298}^{T} \partial \Delta_r \mathbf{G} = -\int_{298}^{T} \Delta_r \mathbf{S} d\mathbf{T} \rightarrow \Delta_r \mathbf{G}_{\mathrm{T}}^{\mathrm{o}} = \Delta_r \mathbf{G}_{298}^{\mathrm{o}} - \int_{298}^{T} \Delta_r \mathbf{S} d\mathbf{T}$$

Method 3. Using the Gibbs-Helmholtz equation:

$$\frac{\Delta_{\rm r}G_{\rm T}^{\circ}}{\rm T} = \frac{\Delta_{\rm r}G_{298}^{\circ}}{298} - \int_{298}^{\rm T} \frac{\Delta_{\rm r}H_{\rm T}^{\circ}}{\rm T^2} \, \mathrm{dT}$$
(3.7)

We also set up equation (3.7) as follows:

Take the derivative of the function $(\frac{G}{T})$ with respect to T:

$$\frac{d}{dT} \left(\frac{G}{T} \right) = \left(\frac{G}{T} \right)^{'}$$
$$\left(\frac{G}{T} \right)^{'} = \frac{G' \times T - T' \times G}{T^{2}}$$
$$\left(\frac{G}{T} \right)^{'} = \frac{G' \times T - G}{T^{2}}$$

Substituting G' = -S (from 3.6) and G = H - TS into the above equation, we get:

$$\left(\frac{G}{T}\right) = \frac{\cancel{BT} - H + \cancel{TS}}{T^2} = \frac{-H}{T^2}$$

Or for chemical reactions:

$$\left(\frac{\Delta G}{T}\right) = \frac{-\Delta H}{T^2}$$
(3.8)

Separating the variables and then integrating equation (3.8), we get:

$$\frac{\Delta_{\rm r}G_{\rm T}^{\rm o}}{T} = \frac{\Delta_{\rm r}G_{298}^{\rm o}}{298} - \int_{298}^{\rm T} \frac{\Delta_{\rm r}H_{\rm T}^{\rm o}}{T^2} \, dT \tag{3.7}$$

In the simple case that the enthalpy variation of reactions does not depend on temperature, the integration of equation (3.7) will be:

$$\frac{\Delta_{\rm r}G_{\rm T}^{\rm o}}{\rm T} = \frac{\Delta_{\rm r}G_{298}^{\rm o}}{298} + \Delta_{\rm r}H_{298}^{\rm o} \times \left(\frac{1}{\rm T} - \frac{1}{298}\right)$$
(3.9)

2.4. Project Summary and Evaluation

Consider the problem of ammonia synthesis:

N₂(g) + 3H₂(g)
$$\xrightarrow{\Delta, \text{ pressure}}_{\text{Fe catalyst}} 2\text{NH}_3(g) \Delta_r H_{298}^o = -91.8 \text{ kJ}$$

Thermodynamic values are referenced in the following table:

Table 1. The	ermodynami	c values of	N2,	H ₂ and NH ₃
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$\Delta_{\rm f} H_{298}^{\circ}$ (kJ/mol)	0	0	-46.3
S ^o ₂₉₈ (J/mol)	191.5	131.0	193.0
Cp° 27.80	$6 + 4.26 \times 10^{-3} T$	$27.28 + 3.26 \times 10^{-3} \mathrm{T} + 0.50 \times 10^{5} \mathrm{T}^{-2}$	$29.80 + 25.48{\times}10^{-3}T {-}1.67{\times}10^{5}T^{-2}$

a) Calculate $\Delta_r G_{298}^o$ of the reaction.

b) Construct the equation $\Delta_r H_T^o = f(T), \ \Delta_r S_T^o = f(T).$

c) Construct the equation $\Delta_r G_T^\circ = f(T)$ using three different methods.

d) Calculate $\Delta_r G_T^{\,o}$ of the reaction at 127 °C.

Solution:

a) Calculate $\Delta_r G^o_{298}$ of the reaction

First we calculate 2 values: $\Delta_r H^o_{298}$ and $\Delta_r S^o_{298}$ then calculate $\Delta_r G^o_{298}$.

$$\begin{split} &\Delta_r H^o_{298} = \sum \Delta_f H^o_{298} (\text{products}) - \sum \Delta_f H^o_{298} (\text{reactants}) \ \Delta_r S^o_{298} = \sum S^o_{298} (\text{products}) - \sum S^o_{298} (\text{reactants}) \\ &\Delta_r H^o_{298} = 46.3 \times 2 - 0 \\ &\Delta_r S^o_{298} = 193 \times 2 - (191.5 + 131.0 \times 3) \\ &\Delta_r H^o_{298} = -92.6 \text{ (kJ)} \\ &\Delta_r S^o_{298} = -198.5 \text{ (J)} \end{split}$$

Inferred:

$$\Delta_{\rm r} G_{298}^{\circ} = -92.6 - 298 \times (-198.5 \times 10^{-3})$$

$$\Delta_{\rm r} G_{298}^{\circ} = -33.447 \text{ (kJ)}$$

b) Build the equation: $\Delta_r H_T^o = f(T), \ \Delta_r S_T^o = f(T).$

$$\begin{split} &\Delta_r Cp^\circ = \sum \Delta Cp^\circ(products) - \sum \Delta Cp^\circ(reactants) \\ &\Delta_r Cp^\circ = (29.80 + 25.48 \times 10^{-3} T - 1.67 \times 10^5 T^{-2}) \times 2 - [27.86 + 4.26 \times 10^{-3} T + (27.28 + 3.26 \times 10^{-3} T + 0.50 \times 10^5 T^{-2}) \times 3] \\ &\Delta_r Cp^\circ = -50.1 + 36.92 \times 10^{-3} T - 4.84 \times 10^5 T^{-2} \text{ (J)} \end{split}$$

Apply equation: (1.2) $\Delta_r H_T^o = \Delta_r H_{298}^o + \int_{298}^T \Delta_r C_p dT$

$$\begin{split} &\Delta_{\rm r} {\rm H}_{\rm T}^{\rm o} = -92.6 \times 10^3 + \int_{298}^{1} (-50.1 + 36.92 \times 10^{-3} {\rm T} - 4.84 \times 10^5 {\rm T}^{-2}) d{\rm T} \\ &\Delta_{\rm r} {\rm H}_{\rm T}^{\rm o} = -92.6 \times 10^3 + \int_{298}^{\rm T} (-50.1) d{\rm T} + \int_{298}^{\rm T} (36.92 \times 10^{-3} {\rm T}) d{\rm T} - \int_{298}^{\rm T} (4.84 \times 10^5 {\rm T}^{-2}) d{\rm T} \\ &\Delta_{\rm r} {\rm H}_{\rm T}^{\rm o} = -92.6 \times 10^3 - 50.1 ({\rm T} - 298) + 36.92 \times 10^{-3} \left(\frac{{\rm T}^2}{2} - \frac{298^2}{2} \right) + 4.84 \times 10^5 \left(\frac{1}{{\rm T}} - \frac{1}{298} \right) \\ &\Delta_{\rm r} {\rm H}_{\rm T}^{\rm o} = -80933.7 - 50.1 {\rm T} + 18.46 \times 10^{-3} {\rm T}^2 + 4.84 \times 10^5 {\rm T}^{-1} \end{split}$$

Apply the equation (2.2): $\Delta_r S_T^o = \Delta_r S_{298}^o + \int_{298}^T \frac{\Delta_r C_p dT}{T}$

We have:

$$\frac{\Delta_r Cp^{\circ}}{T} = \frac{-50.1 + 36.92 \times 10^{-3} \times T - 4.84 \times 10^5 \times T^{-2}}{T}$$
$$\frac{\Delta_r Cp^{\circ}}{T} = -50.1 \times T^{-1} + 36.92 \times 10^{-3} - 4.84 \times 10^5 \times T^{-3}$$

Therefore:

$$\begin{split} &\Delta_r S^o_T = \Delta_r S^o_{298} + \int_{298}^T (-50.1 \times T^{-1} + 36.92 \times 10^{-3} - 4.84 \times 10^5 \times T^{-3}) dT \\ &\Delta_r S^o_T = \Delta_r S^o_{298} + \int_{298}^T (-50.1 \times T^{-1}) dT + \int_{298}^T 36.92 \times 10^{-3} dT - \int_{298}^T (4.84 \times 10^5 \times T^{-3}) dT \\ &\Delta_r S^o_T = -198.5 - 50.1 (\ln T - \ln 298) + 36.92 \times 10^{-3} (T - 298) + \frac{4.84 \times 10^5}{2} \left(\frac{1}{T^2} - \frac{1}{298^2}\right) \\ &\Delta_r S^o_T = 73.2 - 50.1 \ln T + 36.92 \times 10^{-3} T + 2.42 \times 10^5 T^{-2} \text{ (J)} \end{split}$$

c) Construct the equation $\Delta_r G_T^\circ = f(T)$ using three different methods:

(1) Use the Gibbs equation: $\Delta_r G^{\circ}_T = \Delta_r H^{\circ}_T - T \Delta_r S^{\circ}_T$

$$\Delta_{\rm r} G_{\rm T}^{\rm o} = -80933.7 - 50.1{\rm T} + 18.46 \times 10^{-3}{\rm T}^{2} + 4.84 \times 10^{5}{\rm T}^{-1} - {\rm T}(73.2 - 50.1{\rm ln}{\rm T} + 36.92 \times 10^{-3}{\rm T} + 2.42 \times 10^{5}{\rm T}^{-2})$$

$$\Delta_{\rm r} G_{\rm T}^{\rm o} = -80933.7 - 123.3{\rm T} - 18.46 \times 10^{-3}{\rm T}^{2} + 2.42 \times 10^{5}{\rm T}^{-1} + 50.1{\rm T} \times {\rm ln}{\rm T}$$

(2) Using the equation (3.1):
$$\Delta_{\rm r} G_{\rm T}^{\rm o} = \Delta_{\rm r} G_{298}^{\rm o} - \int_{298}^{\rm T} \Delta_{\rm r} {\rm Sd}{\rm T}$$

We have:

$$\begin{split} \int_{295}^{T} \Delta_{r} S_{T}^{\circ} dT &= \int_{295}^{T} (73.2 - 50.1 \times \ln T + 36.92 \times 10^{-3} T + 2.42 \times 10^{5} T^{-2}) dT \\ &\int_{295}^{T} \Delta_{r} S_{T}^{\circ} dT = \int_{295}^{T} 73.2 dT - \int_{295}^{T} 50.1 \ln T dT + \int_{295}^{T} 36.92 \times 10^{-3} T dT + \int_{295}^{T} 2.42 \times 10^{5} T^{-2} dT \\ &\int_{295}^{T} \Delta_{r} S_{T}^{\circ} dT = 73.2 (T - 298) - 50.1 [(T \ln T - T) - 298 (\ln 298 - 298)] + \frac{36.92 \times 10^{-3}}{2} (T^{2} - 298^{2}) - 2.42 \times 10^{5} \left(\frac{1}{T} - \frac{1}{298}\right) \\ &\int_{295}^{T} \Delta_{r} S_{T}^{\circ} dT = 123.2 T - 50.1 T \times \ln T + 18.46 \times 10^{-3} T^{2} - 2.42 \times 10^{5} T^{-1} + 47485.825 \\ \text{Therefore:} \\ &\Delta_{r} G_{T}^{\circ} = -33.3 \times 10^{3} - (123.2 T - 50.1 T \times \ln T + 18.46 \times 10^{-3} T^{2} - 2.42 \times 10^{5} T^{-1} + 47485.825) \\ &\Delta_{r} G_{T}^{\circ} = -80932.825 - 123.3 T + 50.1 T \times \ln T - 18.46 \times 10^{-3} T^{2} + 2.42 \times 10^{5} T^{-1} \\ &(3) \text{ Use the Gibbs-Helmholtz equation (3.7): } \frac{\Delta_{r} G_{T}^{\circ}}{T} = \frac{\Delta_{r} G_{298}^{\circ}}{298} - \int_{298}^{T} \frac{\Delta_{r} H_{T}^{\circ}}{T^{2}} dT \end{split}$$

We have:

$$\frac{\Delta_{\rm r} {\rm H}_{\rm T}^{\circ}}{{\rm T}^2} = \frac{(-80933.7 - 50.1 {\rm T} + 18.46 \times 10^{-3} {\rm T}^2 + 4.84 \times 10^5 {\rm T}^{-1})}{{\rm T}^2}$$
$$\frac{\Delta_{\rm r} {\rm H}_{\rm T}^{\circ}}{{\rm T}^2} = -80933.7 {\rm T}^{-2} - 50.1 {\rm T}^{-1} + 18.46 \times 10^{-3} + 4.84 \times 10^5 {\rm T}^{-3}$$

Therefore:

$$\int_{298}^{T} \frac{\Delta_{r} H_{T}^{\circ}}{T^{2}} dT = \int_{298}^{T} (-80933.7 T^{-2} - 50.1 T^{-1} + 18.46 \times 10^{-3} + 4.84 \times 10^{5} T^{-3}) dT$$

$$\int_{298}^{T} \frac{\Delta_{r} H_{T}^{\circ}}{T^{2}} dT = 80933.7 \left(\frac{1}{T} - \frac{1}{298}\right) - 50.1 (\ln T - \ln 298) + 18.46 \times 10^{-3} (T - 298) - \frac{4.84 \times 10^{5}}{2} \left(\frac{1}{T^{2}} - \frac{1}{298^{2}}\right)$$

$$\int_{298}^{T} \frac{\Delta_{r} H_{T}^{\circ}}{T^{2}} dT = 80933.7 T^{-1} - 50.1 \ln T + 18.46 \times 10^{-3} T - 2.42 \times 10^{5} T^{-2} + 10.856$$

So

$$\frac{\Delta_{\rm r} G_{\rm T}^{\,\circ}}{T} = -123.1 - 80933.7 {\rm T}^{-1} + 50.11 {\rm nT} - 18.46 \times 10^{-3} {\rm T} + 2.42 \times 10^{5} {\rm T}^{-2}$$

$$\rightarrow \Delta_{\rm r} G_{\rm T}^{\,\circ} = -80933.7 - 123.1 {\rm T} + 50.1 {\rm T} {\rm lnT} - 18.46 \times 10^{-3} {\rm T}^{2} + 2.42 \times 10^{5} {\rm T}^{-1}$$

d) Calculate $\Delta_r G_T^o$ of the reaction at 127 °C

Substituting T = 400 K into the above equation, we get:

 $\Delta_r G^{o}_{400} = -80933.7 - 123.1 \times 400 + 50.1 \times 400 \times \ln 400 - 18.46 \times 10^{-3} \times 400^2 + 2.42 \times 10^5 \times 400^{-1} \\ \Delta_r G^{o}_{400} = -12533.35 \text{ (J)}$

3. Conclusion

Through designing the CDIO learning project, students have completed some important content of the following thermodynamics topic:

(i) Three state equations have been explicitly established: $\Delta_r H_T^\circ = f(T)$; $\Delta_r S_T^\circ = f(T)$ and $\Delta_r G_T^\circ = f(T)$. Especially for the first time, when constructing the expression: $-\Delta S = \left(\frac{\partial \Delta G}{\partial \Delta T}\right)_P$ and the Gibbs-Helmholtz equation, students used mathematical knowledge

(differential, integral) that is very close and easy to understand, available in the math program studied at universities. That shows the need to integrate interdisciplinary knowledge together in learning and research.

(ii) In some exercises where it is assumed that the enthalpy change of the reaction does not change with temperature ($\Delta_f H_{298}^o = \text{const}$), the Gibbs free energy of the reaction at the temperature being studied is often approximated as:

$$\frac{\Delta_{\mathbf{r}} \mathbf{G}_{\mathrm{T}}^{\circ}}{\mathrm{T}} = \frac{\Delta_{\mathbf{r}} \mathbf{G}_{298}^{\circ}}{298} + \Delta_{\mathbf{r}} \mathbf{H}_{298}^{\circ} \times \left(\frac{1}{\mathrm{T}} - \frac{1}{298}\right)$$

The reason for this is because:

$$\int_{298}^{T} \frac{1}{T^2} dT = -\left(\frac{1}{T} - \frac{1}{298}\right)$$

Therefore, understanding the nature of each formula will help students solve problems in a natural and interesting way.

(iii) Students can use three different methods to calculate the change in Gibbs free energy of a reaction at a certain temperature T.

(iv) A solid relationship between the equilibrium shift of the reversible reaction according to Le Chatelier's principle and the change of the reaction according to the investigated temperature has been determined.

Example for reaction:

N₂(g) + 3H₂(g)
$$\xrightarrow{\Delta, \text{ pressure}}_{\text{Fe catalyst}} 2\text{NH}_3(g) \Delta_r H_{298}^o = -91.8 \, kJ$$

According to Le Chatelier's principle, when the temperature increases, the equilibrium of the above reaction runs in the direction of NH_3 decomposition (reverse direction). This is completely consistent with the results of calculating the values

$$\Delta_r G^o_{400} = -12533.35 \text{ (J)}_{and} \Delta_r G^o_{298} = -33447 \text{ (J)}.$$

The results show that when the temperature increases from 298 K to 400 K, the Gibbs free energy value of the reaction increases. This means that the efficiency of the ammonia synthesis reaction will decrease as the temperature of the system increases. In fact, the most suitable temperature for this reaction is about 450°C.

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Statement of Competing Interests

The Authors have no competing interests.

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