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Xu, H, Li, S, Song, W, Sun, J, Wu, X, Wang, X, Yang, W, Pan, Z and El Rhalibi, A (2020) Thermal perception method of virtual chemistry experiments. Virtual Reality and Intelligent Hardware Journal, 2 (4). pp. 305-315. ISSN 2096-5796

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Virtual Reality & Intelligent Hardware 2020 Vol 2 Issue 4：305—315

•Article•

Thermal perception method of virtual chemistry experiments

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Received: 29 March 2020 **Accepted:** 17 June 2020

Supported by the National Key Research and Development Program of China (2018YFB1004901); Zhejiang Natural Science Fund Project of China (LY20F020019, LQ19F020012, LQ20F020001); Zhejiang Basic Public Welfare Research Project of China (LGF19E050005); and Major Scientific Research Project of Zhejiang Lab (2019MC0AD01).

Citation: Hengwei XU, Siru LI, Wenpeng SONG, Jiajun SUN, Xinli WU, Xiaoqi WANG, Wenzhen YANG, Zhigeng PAN, Abdennour EI RHALIBI. Thermal perception method of virtual chemistry experiments. Virtual Reality & Intelligent Hardware, 2020, 2(4): 305—315

DOI: 10.1016/j.vrih.2020.07.003

Abstract Background With the aim of addressing the difficulty in identifying temperatures in virtual chemistry experiments, we propose a temperature-sensing simulation method of virtual chemistry experiments. **Methods** We construct a virtual chemistry experiment temperature simulation platform, based on which a wearable temperature generation device is developed. The typical middle school virtual experiments of concentrated sulfuric acid dilution and ammonium nitrate dissolution are conducted to verify the actual effect of the device. **Results** The platform is capable to indicate near real-world experimental situations. The performance of the device not only meets the temperature sensing characteristics of human skin, but also matches the temperature change of virtual chemistry experiments in real-time. **Conclusions** It is demonstrated that this temperature-sensing simulation method can represent exothermic or endothermic chemistry experiments, which is beneficial for students to gain understanding of the principles of thermal energy transformation in chemical reactions, thus avoiding the danger that may be posed in the course of traditional teaching of chemistry experiments effectively. Although this method does not have a convenient enough operation for users, the immersion of virtual chemical experiments can be enhanced.

Keywords Virtual reality; Chemistry experiment; Thermal simulation; Temperature feedback

1 Introduction

Chemistry experiments are crucial in teaching the subject to students thoroughly[1]. By demonstrating exothermic and endothermic processes, some chemical experiments, such as concentrated sulfuric acid dilution experiments, ammonium nitrate dissolution experiments, and liquid nitrogen vaporization latent heat experiments can make students better understand the scientific principles of chemical reactions

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occurring between different substances that involve the conversion of thermal energy. However, in the traditional context of experimental teaching, such experiments are frequently accompanied by a high level of safety risks. If students make mistakes in handling chemicals or experimental equipment, it is highly likely for them to suffer burns or freezing of their skin, resulting in serious injuries. In order to ensure the safety of students while conducting chemical experiments, current regulations prohibit teachers from demonstrating experiments when delivering lectures. In addition, students are forbidden from doing experiments without supervision. As a consequence, students are unable to develop hands-on capabilities to conduct such experiments, which means they cannot intuitively experience the phenomenon of heat absorption in such experiments. This makes it difficult for students to gain a clear understanding about the scientific principle of thermal energy conversion involved in the experiments[2].

For this reason, many studies have focused on virtual chemistry experimental environments and temperature sensing methods[3–5]. Hao et al. applied HTML5 technology to develop virtual physics and chemistry experiments in different middle schools[6]. They relied on geometric modeling and physical characteristics modeling to construct 3D models of experimental equipment, and added them to the virtual experimental scene. Then, they carried out virtual experiments and evaluated experimental results. According to their results, these virtual experiments can be conducted in a browser with a high degree of simulation and close interaction. Zhang et al. developed a middle school chemistry virtual experiment platform using Flash3D[7]. This platform is easily expandable, and capable of connecting to a database for obtaining functions such as experimental teaching, operation, report, and evaluation. Chen et al. constructed a virtual experiment scene and realized human-computer interaction function in virtual chemistry experiments using Kinect somatosensory equipment[8]. Zhang et al. designed a set of immersive virtual chemistry experiment systems based on Untiy3D using virtual reality technology and natural human-computer interaction technology[9].

Despite the capability of these methods to build virtual environments for chemistry experiments, they do not let the experimenter experience temperature changes during the experiments. The results obtained by Ho et al. have revealed that temperature information plays a crucial role in the perception and recognition of people towards objects, which provides a theoretical basis for the necessity to devise a temperature sensing method for virtual chemistry experiments[10]. Citerin et al. developed a device with motion and temperature feedback, which is capable of indicating the kinematics and heat sense calculated by the operator and the 3D virtual environment simultaneously[11]. However, there are shocks in the response of peculiar insulating materials, and the operator is not subject to psychological tests for the evaluation of their perceived performance. Wu et al. developed a rapid surface temperature signal generation device applicable to temperature tactile reproduction, and suitable on other scenarios where rapid changes in surface temperatures is required[12]. Wang et al. designed a temperature tactile presentation device comprising four 15mm×15mm Peltiers that can indicate various temperature changes[13]. Ranasinghe et al. developed a device suitable for gaming, which allows users to feel wind, smell, and temperature changes[14]. They evaluated the impact of different modalities on the virtual experience. Nevertheless, there is no such practical device in the field of virtual chemistry experiments. User evaluation studies of virtual chemistry experiments have also not been conducted.

Therefore, in order to solve many problems in traditional middle school chemistry experiments, especially the problem of temperature perception during chemistry experiments, a temperature sensing method is proposed in this study for virtual chemistry experiments based on virtual reality (VR). It allows students to experience heat absorption and exothermic phenomenon in chemical reactions in real time over the course of experiment, which is conducive in inspiring learning interests of students.

2 Temperature simulation platform of the virtual chemistry experiment

2.1 The overall structure of the simulation platform

The temperature simulation platform designed for virtual chemistry experiments involves a virtual experimental scene, human-computer interaction, and temperature presentation. The virtual experimental scene requires virtual experimental equipment, experimental chemicals, and tools. The user is allowed to observe the virtual chemical experiment scene using the VR head-mounted display device. Moreover, the basic operation of chemical experiments such as pouring water and stirring can be realized through the human-computer interaction module. The temperature presentation module can indicate the temperature in real-time as the chemical reaction proceeds, thus allowing the experimenter to get a sense of how the temperature changes. The overall structure of the platform is illustrated in Figure 1.

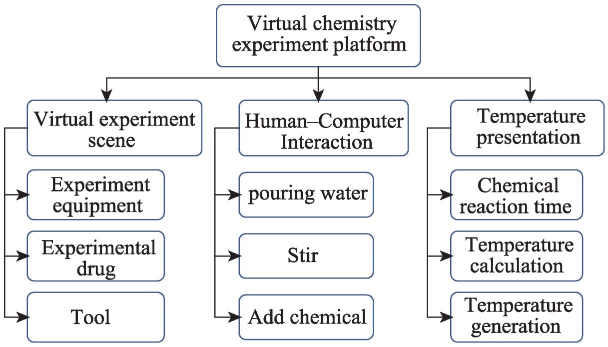
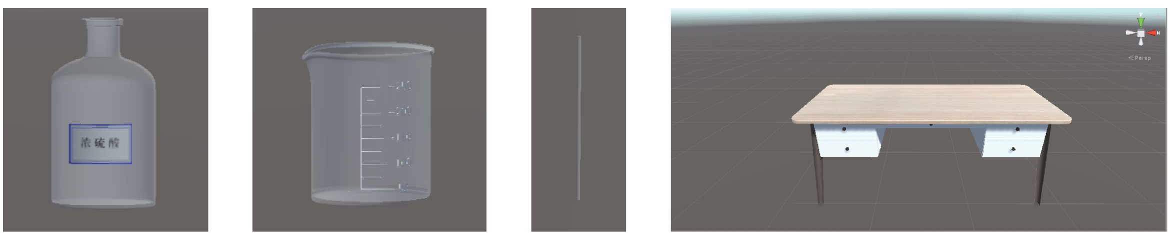


Figure 1 Virtual chemical experiment temperature simulation platform.

We take the concentrated sulfuric acid dilution virtual experiment as an example. Firstly, experimental equipment such as glass bottles, beakers, glass rods, and test benches are constructed. Secondly, the virtual experimental scenes such as light rendering and glass collision sound effects are set up. Then, the human-computer interaction operation is designed for the concentrated sulfuric acid dilution experiment. Concentrated sulfuric acid is poured into a beaker filled with water at a slow pace, while a glass rod is used to stir the solution uniformly. Finally, the change in temperature of exothermic dilution with concentrated sulfuric acid are shown.

2.2 Construction of the virtual experiment scene

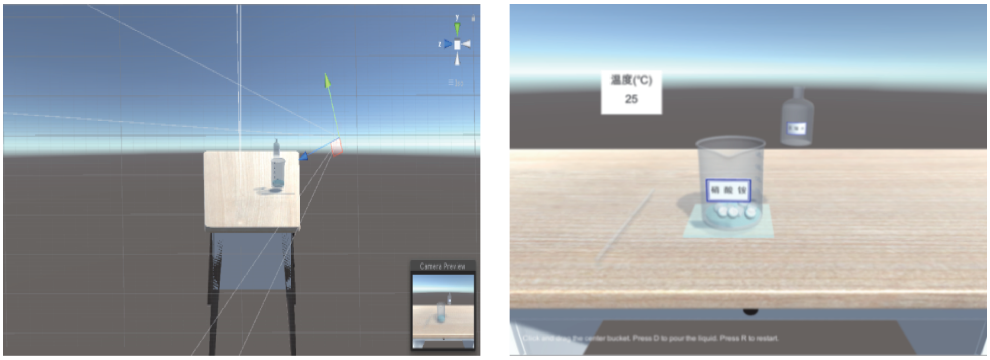
Firstly, 3D models were constructed for beakers, glass bottles, glass rods, and test benches in 3DMAX, before being saved as FBX files and inputted into Unity3D, where the experimental instruments were labeled, and the corresponding materials were added. After the materials were rendered, experimental instruments with real texture were obtained. Some appliance models are shown in Figure 2.



(a) Glass bottle (b) Beaker (c) Glass rod (d) Test bench

Figure 2 Experimental instrument models.

Then, C# language was applied in in Unity3D to create a virtual experimental scene, including the lighting layout, main camera position, experimental chemicals, and water model production. Figure 3 shows a rendered scene of the virtual chemical experiment.



(a) The location of the main camera (b) Laboratory equipment and experimental chemicals

Figure 3 Scene of the virtual chemistry experiment.

2.3 Platform function module

2.3.1 Human-computer interaction module

The human-computer interaction modules mainly involves glass rod stirring and glass bottle pouring. In the Unity3D animation control panel, animation components were added into the experimental equipment model, rotation key frames were introduced, the animation curve was modified, the movement of each model was subjected to control, and a script program was written. Finally, human-computer interaction was realized. Because this experiment needs users to use a constant speed to pour and stir water, we assigned different keyboard buttons to control these experimental equipment.

2.3.2 Sound module

The sound effect file was added into the audio playback component of the experimental equipment model before a script was written. When the experimental equipment is operated through human-computer interaction, the sound effect file can be triggered and played to generate a realistic sound.

2.3.3 Particle module

The Shuriken particle system was applied to generate random water-like particles in a glass bottle. A script was used to plan the flow dump path, while allowing the particle effects to move through the path to simulate the flow of water.

2.3.4 Temperature generation module

During the experiment, a script was used to impose control on the changes in temperature. Visually, a digital display was employed to show how the temperature would change, and a wearable temperature generating device was used to sense how the temperature changes.

The above-mentioned modules work together to achieve temperature sensing in virtual chemistry experiments.

3 Wearable temperature generating device

3.1 Structure of the device

In this study, we develop a wearable temperature generating device featuring wireless communication, digital-to-analog conversion, and cold and heat conversion, as shown in Figure 4. This device relies on Peltiers (model TEC1-12706) to realize temperature generation. As a current-transducing device, a Peltier can increase or reduce the temperature quickly, and regulate the temperature change accurately. Moreover, it has a large temperature change interval and long service life.

The wearable temperature generating device consists of a host and a slave. The host contains a Bluetooth module, battery, processor, etc., which can be worn on the arm. The slave device contains relay circuit boards, Peltiers, etc. While functioning, the host communicates with the computer via Bluetooth, and the main control chip of the processor (model Mega2560) processes the temperature command received from the computer before sending it to the relay circuit of the slave to drive the Peltiers. The structure of the device is shown in Figure 5.

Figure 4 Wearable temperature generation device.

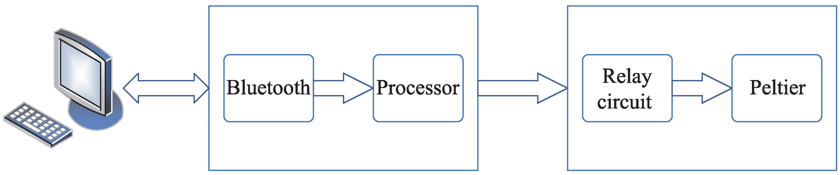


Figure 5 Structure of the wearable temperature generation device.

3.2 The workflow of the device

The working flowchart of the proposed device is presented in Figure 6. The upper computer (1) displays the scene of the virtual chemistry experiment, while the temperature command of the scene is sent to the lower computer control platform (3), via the Bluetooth communication module (6), according to the set communication protocol. After recognizing and decoding the temperature command, the lower computer control platform converts it into a transistor-transistor logic signal of the I/O port, and transmits it to the Peltier drive module (4). As a result, the Peltier module (5) generates temperature changes. The temperature sensing module (8) measures the temperature of the Peltier module, and displays it in the temperature display module (7). The battery module (2) is responsible for powering all the electronic components in the device.

For example, when a scene of heating a beaker with an alcohol lamp appears in a virtual chemistry experiment, the script program of the scene calculates that the temperature of the solution in the beaker is 50℃, with 50℃ displayed in the virtual chemistry experiment scene of the host computer. The upper computer issues a temperature instruction to the lower computer control platform through the Bluetooth communication module, after which the Peltier module heats up. The temperature sensing module is in place to monitor the indicated temperature of the Peltier module in real-time. The Peltier module continues to heating if the temperature is lower than 50℃, after which the Peltier module stops heating.

The temperature generating function of the device involves a Peltier drive module and a Peltier module. The schematic diagram of the circuit connection is shown in Figure 7. The Peltier driver module contains a DC motor driver chip that is connected to the lower computer control platform through the chip pins. The Peltier module contains two Peltier chips.

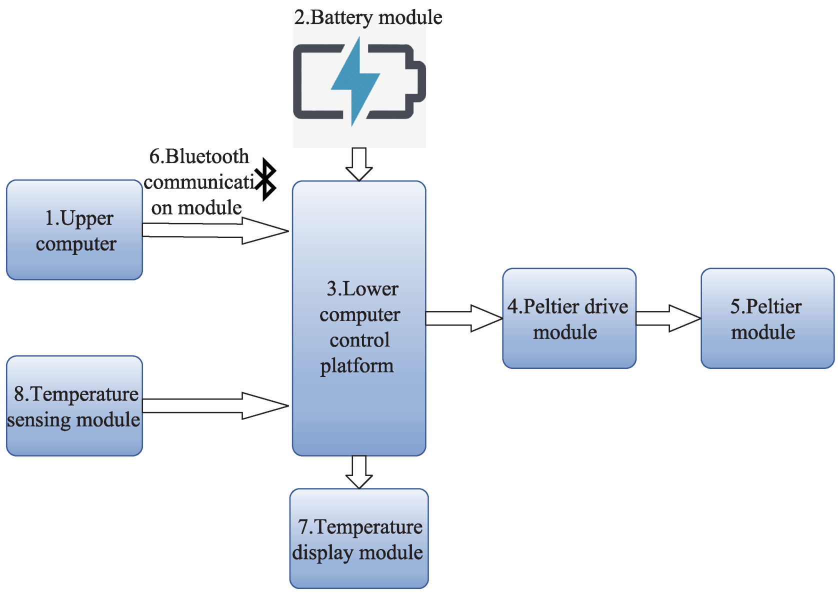


Figure 6 Work process of the wearable temperature generation device.

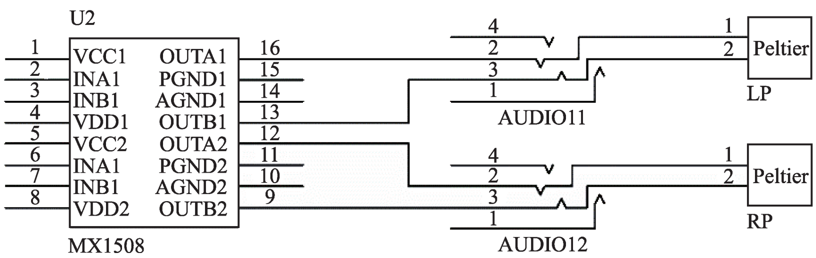


Figure 7 Circuit diagram of the Peltier drive module.

3.3 Device performance

In order to determine the temperature change of the device, a surface thermo-couple thermometer (model hy101k) was employed to measure the temperature change of the device at room temperature (26℃). The curves of temperature change over time are shown in Figures 8 and 9, respectively.

$$\Delta T_{rise} = T - 26 \tag{1}$$

$$\Delta T_{fall} = 26 - T \tag{2}$$

Here, T represents the measured temperature in the thermometer, ΔT_{rise} indicates the absolute value of the temperature rise, and ΔT_{fall} denotes the absolute value of the temperature drop.

As shown in Figures 8 and 9, during the period between 0–10s, the values of ΔT_{rise} and ΔT_{fall} change rapidly, suggesting that the device can heat up or cool down at a fast pace. It can match temperature changes in chemistry experiments in real time. It was also found that between 0–10s, both ΔT_{rise} and ΔT_{fall} are sufficiently large. The temperature change per second can reach ±2℃, which indicates that the temperature change of this device can make heating and cooling perceptible for human skin, which is consistent with

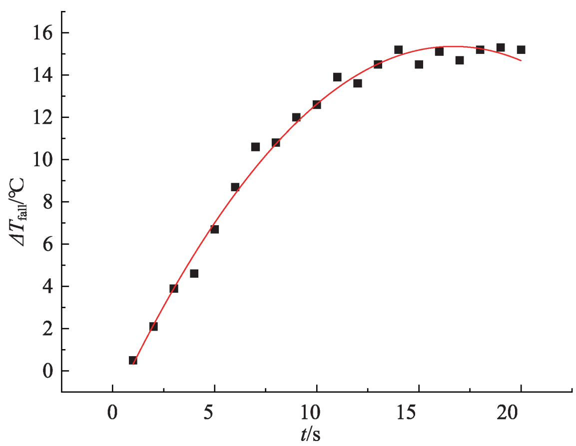


Figure 8 Temperature curve of the cooling process.

the resolution of the perception that skin has towards temperature changes. The temperature of the device ranges between −4℃ and 53℃, which indicates that the device will not cause freezing or burning to skin, and therefore, it is deemed safe. As the working time is extended, the changes in the values of ΔT_{rise} and ΔT_{fall} are small, especially between 15−20s, when the cooling effect is insignificant. This implies that our device is unfit for prolonged usage. After 15s of functioning, the power supply must be halted.

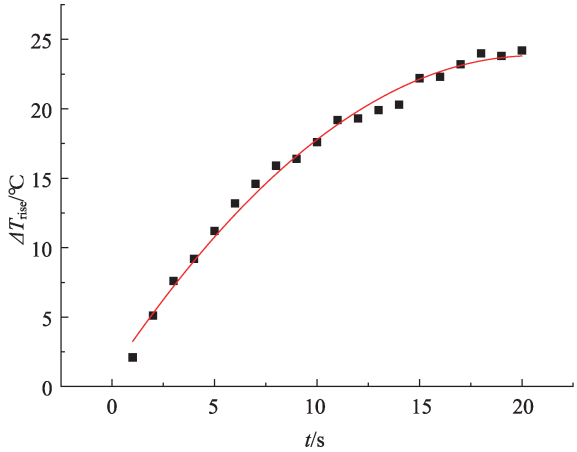


Figure 9 Temperature curve of the heating process.

4 Experimental verification

The platform and the devices are applied to middle school virtual chemistry experiments. The experimental flowchart for users is shown in Figure 10.

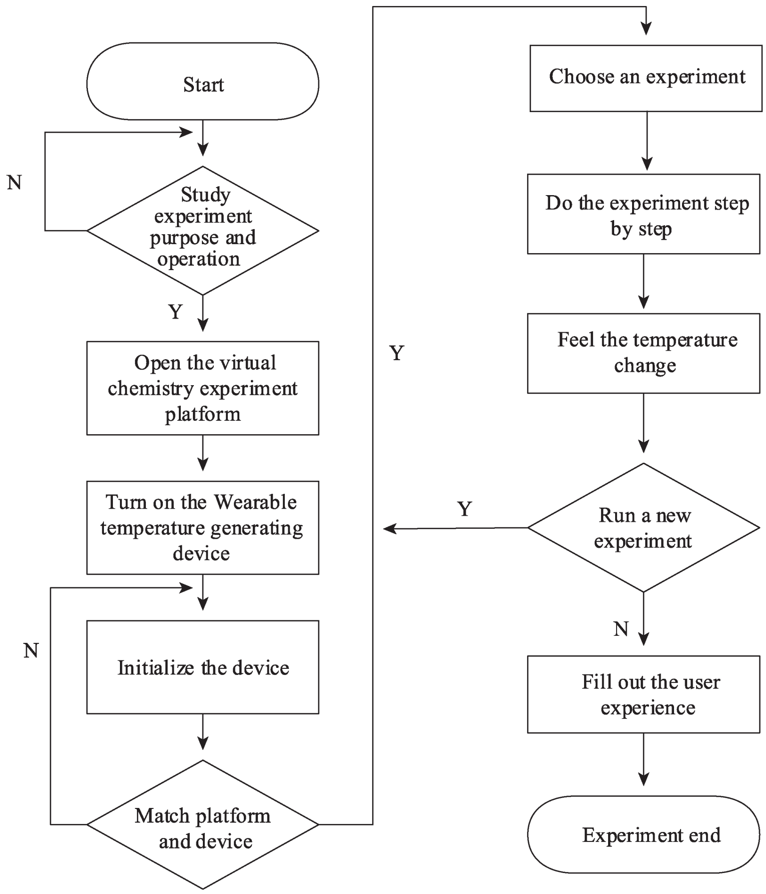


Figure 10 Experimental flowchart for users.

In order to establish whether this method is effective in making students perceive endothermic and exothermic processes in virtual chemistry experiments, experimental research was conducted on the user experience. Forty science students participated in the experimental study, including 20 boys and 20 girls, all of whom were third-year students at our university (average age 20). They had never conducted similar experiments.

4.1 Diluted VR experiment with concentrated sulfuric acid

Based on the characteristics of the concentrated sulfuric acid dilution experiment and the working performance of the wearable temperature generating device, the temperature change of the device was simulated after different amounts of concentrated sulfuric acid were poured into the beaker during the concentrated sulfuric acid dilution VR experiment. For safety purposes, heating was discontinued when the temperature of the device reached 49.8℃. Table 1 indicates the corresponding relationship between the temperature value of the actual experiment of concentrated sulfuric acid dilution, and the temperature value generated by the device. Despite the same trend of the temperature rise, the device temperature and real experimental temperature are not the same.

Table 1 The relationship between the temperature value of concentrated sulfuric acid dilution physical experiment and the temperature value generated by the device

Capacity/mL	Time/s	Temperature/℃	Device temperature/℃
0	0	26	26
5	6	63.5	35.65
6	8	67.8	36.8
7	9	73	38.2
8	10	76.3	44.4
9	12	80.2	45.3
10	13	83.7	49.8
15	20	96.4	49.8

4.1.1 VR experimental design and process

Prior to the experiment, the experimenters were briefed on the purpose and operation of the VR experiment with concentrated sulfuric acid dilution. Then, the experimenters were instructed to put on the temperature generating device, and complete the experiment individually. After the experiment, the experimenters were required to fill in a questionnaire, and the questionnaire data were later analyzed.

At a room temperature of 26℃, the experimenters slowly poured 15mL of concentrated sulfuric acid with a concentration of 98% into 20mL of water along the walls of the beaker, which was accompanied by continuous stirring using a glass rod. As observed by the experimenters, the temperature of the solution in the beaker kept increasing when the concentrated sulfuric acid was poured into the beaker.

As shown in Figure 11, the experimenters opened the temperature simulation platform of the virtual chemistry experiment, connected Bluetooth, and wore the temperature generating device on both hands to conduct the experiment. The experimenters poured concentrated sulfuric acid into a beaker of water, stirred the solution with a glass rod, and perceived the temperature change occurring to the concentrated sulfuric acid.

(a) Experimental scene (b) Experimenter operation

Figure 11 Concentrated sulfuric acid dilution VR experiment.

During the experiment, the experimenters can watch the temperature value rise continuously, as indicated by the temperature value displayed on the screen. In the meantime, the platform issues a temperature command to the wearable temperature generating device through the Bluetooth connection.

The skin on the back of the hands of the experimenters sense the temperature increase when the concentrated sulfuric acid is diluted.

4.1.2 User experience evaluation

In the traditional context of teaching chemistry experiments, the concentrated sulfuric acid dilution experiment is considered to be highly dangerous, which can easily lead to accidents. Most schools prohibit students from doing this experiment without supervision. During the VR experiment of concentrated sulfuric acid dilution, the temperature simulation platform of the virtual chemistry experiment can represent the concentrated sulfuric acid dilution experiment scene accurately. In addition, the wearable temperature generating device allows students to sense the temperature change of the solution through their skin when concentrated sulfuric acid is diluted.

A majority of the experimenters admitted that they could easily sense the temperature rise during the VR experiment of dilute sulfuric acid. Compared with the actual experiment of concentrated sulfuric acid dilution, the experimenters considered the concentrated sulfuric acid dilution VR experiment as more attractive, and the exothermic phenomenon of concentrated sulfuric acid dilution as impressive. According to the statistical results of the questionnaire survey, the VR experiment of concentrated sulfuric acid dilution demonstrated safety, authenticity and interaction. Table 2 details the statistical results of the user experience.

Table 2 User experience of concentrated sulfuric acid dilution VR experiments

Evaluation project	Heating rate		Temperature feeling			Temperature rise obvious		Compared with traditional experiments		
Evaluation results	Fast	Slow	Feeling hot	No feeling	Feeling cold	Yes	No	Better	Same	Worse
Number of people	36	4	38	2	0	37	3	33	3	4

4.2 Ammonium nitrate dissolution VR chemical experiment

Based on the characteristics of the actual experiment of ammonium nitrate dissolution with regard to temperature change and the performance of the wearable temperature generating device, the temperature changes of the device were simulated after different amounts of water were poured into the beaker during the VR experiment of ammonium nitrate dissolution. When the temperature of the device reached 9.8℃, the device discontinued the process of cooling down. Table 3 shows the corresponding relationship between the temperature of the actual experiment of ammonium nitrate dissolution and the temperature generated by the device. The two exhibit the same trend of cooling, although the absolute temperature being different.

4.2.1 VR experimental design and process

Prior to the experiment, the experimenters were informed about the purpose and operation of the ammonium nitrate dissolution VR experiment. Then, the experimenters were required to wear the temperature generating device before completing the experiment individually. Following the experiment, the experimenter was asked to fill in the questionnaire. Subsequently, the questionnaire data were analyzed.

Table 3 Relationship between the temperature value of ammonium nitrate dissolution physical experiment and the temperature value generated by the device

Capacity/mL	Time/s	Temperature/℃	Device temperature/℃
0	0	25	25
5	5	24.8	18.3
10	10	23.7	12.4
12	12	23.6	11.4
14	14	23.4	9.8
16	16	18	9.9
18	18	16.2	9.8
20	20	14.8	9.8

As shown in Figure 12, the experimenters opened the temperature simulation platform of the virtual chemistry experiment, connected Bluetooth, and wore the temperature generating device on both hands to conduct the experiment. At 26℃, 16mL of water was slowly poured into a beaker containing 30g of solid ammonium nitrate, while the solution was continuously stirred with a glass rod. The experimenters could sense that the temperature of the solution in the beaker continued to drop as the ammonium nitrate dissolved.

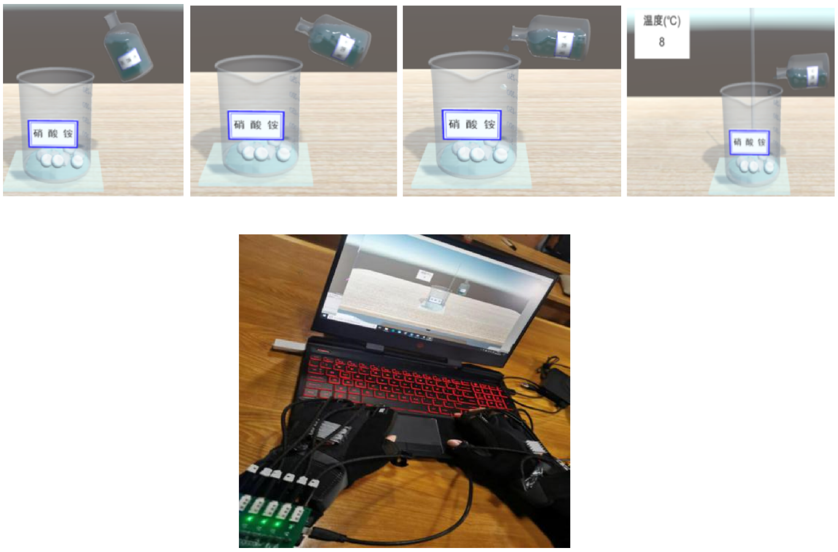


Figure 12 Ammonium nitrate dissolution VR experiment.

During the course of the experiment, the experimenters could see the temperature continue on a decreasing trend on the screen. At the same time, the platform issued a temperature command to the wearable temperature generating device through the Bluetooth connection. The skin on the back of the hands of the experimenters could sense the decrease in temperature. Therefore, the endothermic phenomenon could be experienced as ammonium nitrate dissolved.

4.2.2 User experience evaluation

During the VR experiment of ammonium nitrate dissolution, the temperature simulation platform of the virtual chemistry experiment could represent the ammonium nitrate dissolution experiment scene accurately. In addition, the wearable temperature generating device allowed students to sense the change in temperature of the solution ease when the ammonium nitrate dissolved. As revealed by the statistical results of the questionnaire survey, the VR experiment of ammonium nitrate dissolution also demonstrates excellent science, safety, authenticity, and interaction. The statistical results of user experience are presented in Table 4.

Table 4 User experience of ammonium nitrate dissolution VR experiment

Evaluation project	Cooling rate		Temperature feeling			Temperature fall obvious		Compared with traditional experiments		
Evaluation results	Fast	Slow	Feeling hot	No feeling	Feeling cold	Yes	No	Better	Same	Worse
Number of people	39	1	0	4	36	37	3	34	3	3

In general, experimenters considered that in the VR experiment of ammonium nitrate dissolution, their skin could sense the fast-paced drop of temperature with ease, which is interesting, and prompted them to think deeply about the scientific principle behind the endothermic phenomenon of ammonium nitrate dissolution.

5 Conclusion

In this study, we propose a thermal perception method of virtual chemistry experiments based on VR, and conducted user experience research concentrated sulfuric acid dilution VR experiment and ammonium nitrate dissolution VR experiment to validate the effectiveness of the proposed method. According to the experimental results, this method can assist in carrying out virtual chemistry experiments through natural human-computer interaction, and allow students to sense endothermic and exothermic phenomena in the course of virtual chemistry experiments through their skin, which addresses various shortcomings of traditional chemical experiments.

Moreover, a temperature simulation platform of virtual chemistry experiments is constructed, which is capable of carrying out multiple virtual chemistry experiments, thus showing its generality to some extent. Furthermore, a wearable temperature generating device is designed, the working performance of which is validated by the verification by students that their skin could sense the temperature change in chemical reactions. Although the Peltier has fast response to the change in temperature, a small delay between them is observed from our experiments. This difference shall be analyzed to improve the immersion of virtual chemical experiments.

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