The Virtual Chemical Laboratory Using Particle and Volume Based Liquid Model

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***Abstract*—We have researched an interactive manipulation model of virtual liquid. Representing a vortex, a spinning flow of liquid, simulating a stirring action of liquid, and coloring of the water object through changing the surface color has been developed. In this paper we propose a VR chemical laboratory system using these techniques. This system can be used for different kind of purposes, for example e-learning. E-learning offers potentially cheaper education, increased accessibility and convenience for users. Most existing systems rely on transmitting information through text material, but by adding virtual reality content to the system the learning experience can surely be improved.**

I. Introduction

Creating realistic looking liquids in realtime that can be interacted with is a challenging problem. Highly accurate models using methods such as the Navier-Stokes equations can be used for achieving realistic liquids, but are as for now unpractical for realtime simulations without specialized hardware or e.g. GPU calculation [1][2][3][4].

On the other hand, simplified models are needed for creating realtime liquid simulations which can be used for applications that do not need a high degree of realism, such as experience systems and games, with restricted hardware. A particle and volume based liquid model is proposed, which enables manipulation of virtual liquid with high processing speed [5]. The interaction between containers and liquid is considered. The features of the motion of liquid which humans expect unconsciously is mainly represented. So we can manipulate virtual liquid in the highly feeling of liquid manipulation. In addition, virtual liquid model to focus waves and splash of the liquid surface, or to represent coloring is proposed [6][7][8]. These models avoid complex calculation for realizing the realtime simulation.

Our work focuses on a VR laboratory system which could be used e.g. for e-learning or games, and is based on particle and volume based liquid models. We propose a model which represents color diffusion inside the liquid and a vortex created by stirring for VR chemical laboratory systems. The system uses a simplified model for representing the liquid, rendering and interactively manipulating it. For this kind of an application our criteria has been to make a model which is able to represent interaction between two or more liquids, e.g. when two liquids are mixed in one container, since mixing liquids is a common operation in chemistry experiments. In section II a particle and a liquid based models are outlined, section III outlines the method for the liquid surface's diffusion and coloring, section IV outlines the stirring motion and the vortex that occurs and section V outlines the results of the developed system.

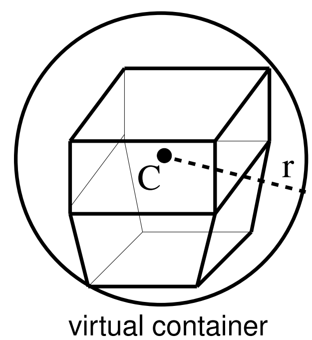

Fig. 1. Virtual container inside a bounding sphere

II. Particle and Volume Based Model

In this section, particle and volume based interactive liquid manipulation models are described which is the foundation of our work.

A. Virtual Container

For manipulating virtual liquid, we use a virtual container. The virtual container is inside a bounding sphere and is used for detecting the interference (Fig. 1). The center of the sphere is designated as $\mathbf{C}$ and its radius is designated as $\mathbf{r}$. The position of a virtual container is represented by $\mathbf{C}$. Inclination and direction of a virtual container is represented by θ, ϕ, and ψ (Fig. 2). A virtual container is rotated by ϕ on axis x_c, and rotated by θ on axis z_c. In short, the tilt parameters are represented by θ and ϕ. Then a virtual container is rotated by ψ on axis y_c and its direction is changed.

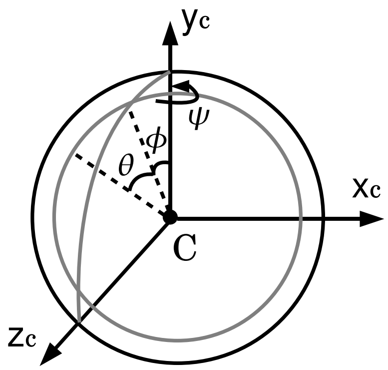

Fig. 2. Representation of tilting of virtual containers

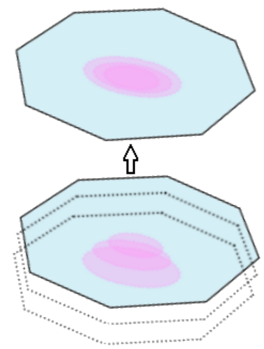

Fig. 3. Multiple layers of grids for representing coloring

B. The liquid model

Using purely a particle based system in three dimensions using many particles the calculations become too heavy. This is the reason the liquid in the presented system is represented with a volume and a particle based system. In this system, we can manipulate virtual liquid using a container mentioned above, e.g. by spilling and ladling. Although this model doesn't calculate the motion of liquid precisely, it represents features of the motion of liquid which the human naturally expect. It enables us to feel that the virtual liquid is real.

1) Particle based liquid: A particle system is used for representing liquid in free fall. Interaction between the particles does not happen, but once a particle hits a volume liquid it increases its volume by one unit. The particle is converted into volume according to the rate of convertion N[number of particle / cc]. For instance, when the particles which is the number of N times V collide with the volume based liquid, the volume of V is increased.

2) Volume based liquid: The volume based system is used for liquids that are accumulated in e.g. containers. A volume of liquid in our proposed model is a three-dimensional object with an upper surface and several side surfaces. The upper surface is deformable and is represented with a height grid and can be manipulated and interacted with. A two-dimensional wave equation (eq. 1) is used. The value v means the speed of the wave.

$$\frac{\partial^2 z}{\partial t^2} = v^2(\frac{\partial^2 z}{\partial z^2} + \frac{\partial^2 z}{\partial y^2}) \tag{1}$$

The following equation is derived from (eq. 1), and is used for calculating the height h of the grid point (i, j) at time t+Δt.

$$\begin{aligned} h[i][j](t+\Delta t) &= ((h[i+1][j](t) + h[i-1][j](t) \\ &\quad + h[i][j+1](t) + h[i][j-1](t))/2 \\ &\quad - h[i][j](t-\Delta t)) \times c \end{aligned} \tag{2}$$

The value c means damping coefficient, which gives optional consideration for the wave's attenuation. The wave on the liquid surface is represented by calculating transmitting waves on grid points. The surfaces on the sides are static and do not deform.

III. Diffusion and Coloring

When liquids of different colors are poured into the same container in the volume based model, diffusion occurs i.e. the liquids in the container mix. The information of the diffusion is handled in a three dimensional grid (the actual surface is a two dimensional grid, but a multiple layers of grids are used for obtaining a sense of depth (Fig. 3)), and the diffusion happens according to the equation below:

$$\begin{aligned} \frac{\partial P(x,y,z,t)}{\partial t} &= D(\frac{\partial^2 P(x,y,z,t)}{\partial x^2} + \frac{\partial^2 P(x,y,z,t)}{\partial y^2} \\ &\quad + \frac{\partial^2 P(x,y,z,t)}{\partial z^2}) \end{aligned} \tag{3}$$

P denotes the concentration of the liquid at a certain point, and D is the diffusion coefficient. The solution to this equation is calculated numerically, by doing the following calculations on each time step:

$$\begin{aligned} &(C[i][j][k](t+\Delta t) - C[i][j][k](t)) \\ &\times P[i][j][k](t+\Delta t) \times \frac{d^2}{D\Delta t} \\ &\quad = C[i+1][j][k](t) \times P[i+1][j][k](t) \\ &\quad + C[i-1][j][k](t) \times P[i-1][j][k](t) \\ &\quad + C[i][j+1][k](t) \times P[i][j+1][k](t) \\ &\quad + C[i][j-1][k](t) \times P[i][j-1][k](t) \\ &\quad + C[i][j][k+1](t) \times P[i][j][k+1](t) \\ &\quad + C[i][j][k-1](t) \times P[i][j][k-1](t) \\ &\quad - 6P[i][j][k](t) \end{aligned} \tag{4}$$

C contains the color information in RGBA-form, and d is the width of the grid. The difference in P causes a difference in the coloring (Fig. 4). The colors for rendering the upper surface is done in a simple manner. In the experiment section, the two-dimensional array surface[x][y][0], surface[x][y][1] and surface[x][y][2] is used for representing diffusion of color on the liquid surface.

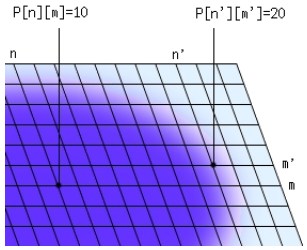

Fig. 4. Coloring with different values of P

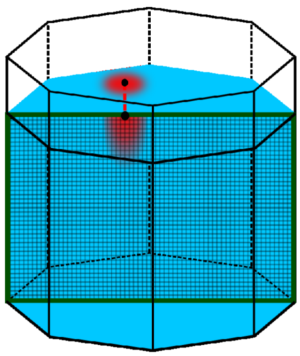

Fig. 5. A slice from the middle of container used for color diffusion

A similar method is used for the side surfaces. A slice from the middle of the container facing the viewer but parallel to the y axis is used for diffusion of color as shown in Fig. 5. The width of this grid which is used for the side projection is $\pi\mathbf{r}$, where $\mathbf{r}$ is the radius of the bounding sphere of the object. Fig. 6 shows how this projection is done. This projection is put onto the surfaces that are visible from the viewpoint and that are facing forward. The length L_j of each side j is calculated with the following formula:

$$L_j = \frac{W_i}{\sum_k W_k} \times \pi\mathbf{r} \tag{5}$$

W_i denotes the length of a polygon and is calculated by the difference of the biggest and smallest x-coordinate. The diffusion is then represented by applying a texture on each polygon of the side surface (Fig. 7).

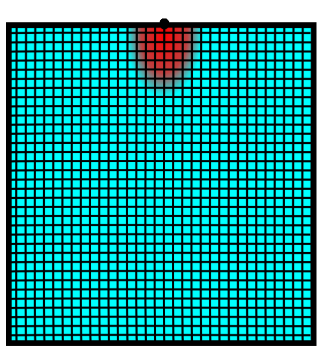

Fig. 6. Diffusion of the color on the projection

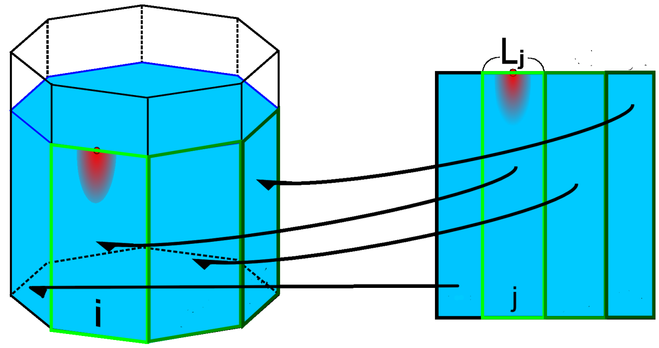

Fig. 7. Putting texture onto the side surface

This is done to save computation time. Instead of making a projection calculation for each surface, only one calculation is made greatly reducing computation time.

IV. VORTEX

Since mixing a liquid is a typical operation in chemistry experiments e.q. by stirring liquids with spoon like objects, its operation is needed in the model of interactive liquid manipulation. Representation of a vortex on liquid surface enables us to stir virtual liquid in high presence. To represent the flow of water precisely like a vortex, calculations which are based on hydrodynamics are necessary, but it needs a lot of computing time, which means that it is not suitable for the interactive manipulation model. Therefore, we represent a vortex which is composed of spiral waves and a depression of the liquid surface So far the meshed surface with grid points is used for representation of the spreading waves on the liquid surface (Fig. 8). In addition, we adopt the surface which have

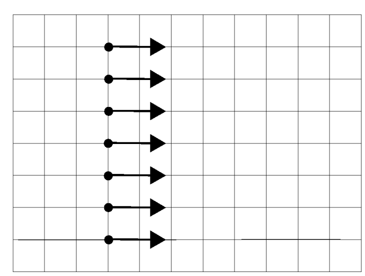

Fig. 8. Spreading waves on the meshed surface

grid points on a concentric circle (Fig. 9). The waves spread on it and the spiral waves is developed (Fig. 10). A depression in the liquid surface is calculated by the following equation.

$$z = \begin{cases} \dfrac{\omega^2}{8g}(r^2 - 2a^2) & (r < a) \\[2ex] \dfrac{\omega^2}{8g}\dfrac{a^4}{r^2} & (r \geq a) \end{cases} \tag{6}$$

The value ω means the power of vortex, r means the length from the center of vortex, g means the gravitational acceleration, and a means the boundary between forced vortex and

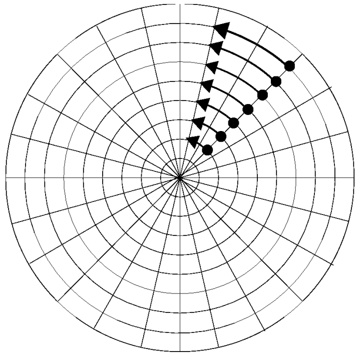

Fig. 9. Spreading waves on the concentric circle surface

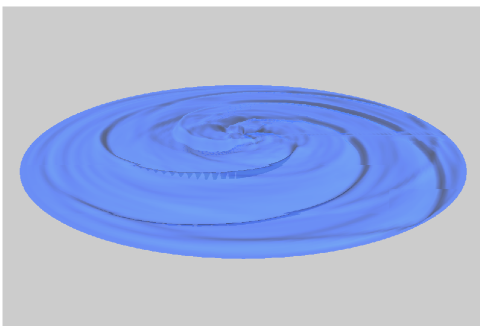

Fig. 10. Spiral waves on the liquid surface

free vortex. The forced vortex and the free vortex are different in the speed of liquid flow. The value of a is the radius of vortex. The size of the vortex is decided from the average location of the object doing the stirring, and ω is decided from the direction and distance of the object's movement in this model. The depression in the liquid surface is shown in Fig. 11 and Fig. 12. Our vortex is done by applying the

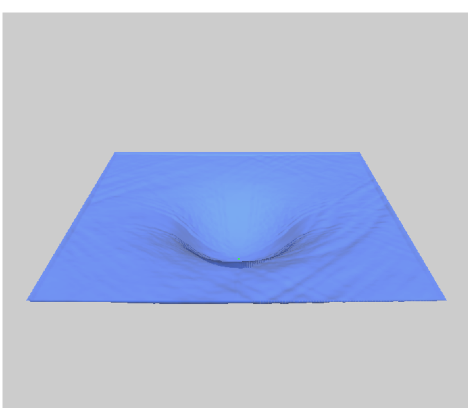

Fig. 11. Depression in the liquid surface

equation 5 on the height of the liquid surface, making the surface appear concave. The vortex is made to form in the center of the container. To increase the strength of the vortex by stirring, we look if the motion of the object doing the stirring is in a clockwise or an anti-clockwise motion and

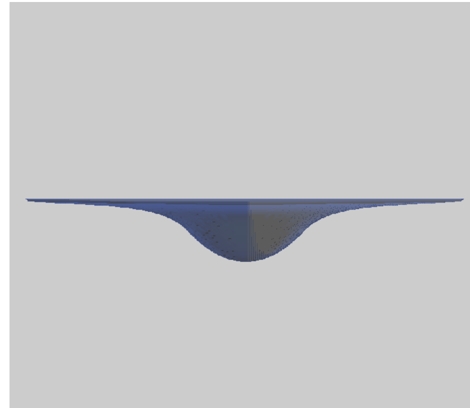

Fig. 12. Depression in the liquid surface (side viewing)

TABLE I
DRAWING UPDATE SPEED OF PROPOSED MODEL

Action performed	Frame rate
No action / idle	60 fps
Pouring liquid	47 fps
Stirring	47 fps

increase ω. If the object moves in an opposite direction of the vortex's direction ω is decreased. If the motion continues in the opposite direction the vortex disappears and a new vortex is formed with the opposite direction. When stirring happens, the diffusion is made faster.

V. EXPERIMENTAL RESULT

The virtual chemical laboratory system using the model mentioned above was implemented with C language. The specification of PC is the following; CPU: Dual-Core AMD Opteron Processor 1210 1.8GHz. The experimental system has containers and/or objects, which one is movable and the other is fixed. The position and the direction of the movable object are input from a real object with the motion sensor using a low-frequently magnetic field. The device we used is 3SPACE ISOTRAK2 of Polhemus company.

In Fig. 13, the state of color diffusing inside of the liquid is shown. Particles which are of white color are dropped into brown water, and then the white color spread. In Fig. 14, the vortex is shown. The spiral waves and depression of the liquid surface gives an impression of stirring. In Fig. 15, simple chemical experiments which is conducted is shown. A chemical experimental tool in the virtual world is manipulated by using tool in the real world. An operater pours a chemical into another chemical, and stir it with a glass stick, and then chemical reaction happens (Fig. 16). The model we proposed enables us to experience chemical experiments with high realism.

The result about processing speed is shown in Table 1. The calculations in the interactive liquid manipulation system has a low cost of computation. Although the interactive manipulation system needs at least 10-12 fps, the model we proposed satisfies it enough.

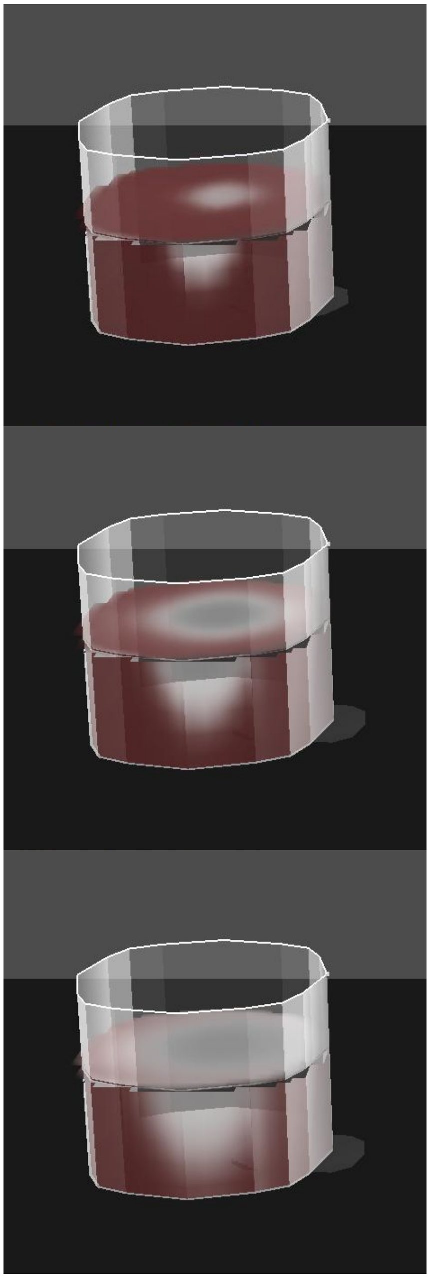

Fig. 13. Color diffusion

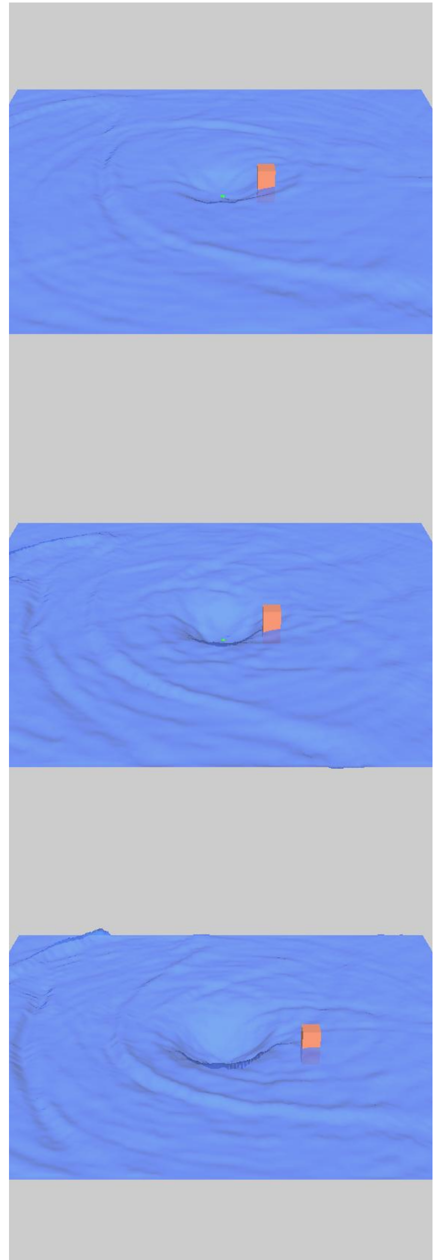

Fig. 14. Stirring liquid and a vortex appears

VI. Conclusion

In this paper, we proposed a virtual chemical laboratory system using methods of diffusing color inside the liquid and representation of a vortex on the liquid surface. These models do not calculate complex processes but enable us to manipulate virtual liquid with high realism. The level of realism of this system is further improved by focussing on the liquid behavior and the shape of containers. The realization of liquid manipulation with concave containers, e.g. glasses which are narrow in the middle and flasks, is one of our solutions. The vortex is not based on hydrodynamics, and this model represents chemical reaction by coloring diffusion. Therefore the differences of the result caused from the factor like temperature can not be expressed. So it is difficult to apply to experiments we do not know the result of. Although it is available for the e-learning systems which use VR technology that have known results. Besides the e-learning system, this model is useful for other applications or systems with interactive manipulation because of its high processing speed. Researching and devising the model for improvement of the feeling of liquid manipulation, e.g. representation of the liquid tricked down container surface, is the subject of our future work.

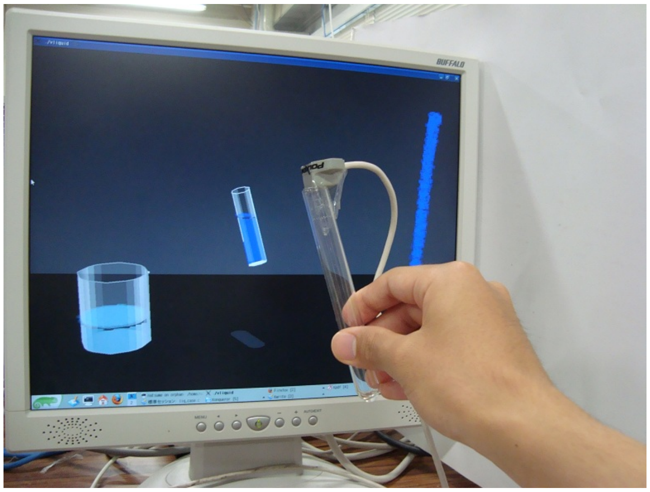

Fig. 15. Using the VR chemical Laboratory

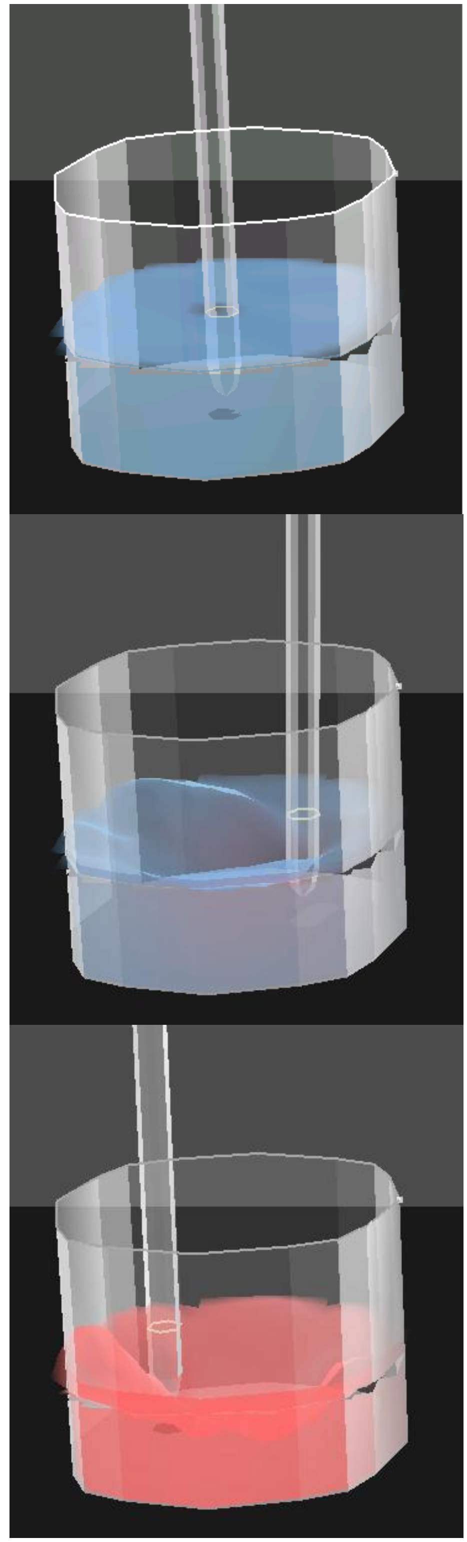

Fig. 16. Stirring chemicals in chemical experiment

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