

Reusable Instant Cooler based on Endothermic Chemical Reactions

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ABSTRACT: Current portable cooling solutions are neither reusable nor truly portable. This paper explores the use of reversible endothermic gaseous chemical reactions to create a truly portable, reusable instant cooler that is human powered. While there are multiple use cases, the paper describes mathematical modelling of a beverage cooling system. This mathematical modelling takes into account various high level chemistry concepts like thermodynamics, chemical kinetics, and chemical equilibrium. This analysis provides a complex system of non-linear differential equations, which can be solved to identify the feasibility and favourable conditions under which such a system can operate.

KEYWORDS: Reusable, Instant cooler, Endothermic Reactions, Chemical Kinetics, Thermodynamics, Portable Cooler

I. INTRODUCTION

Cooling sensations are strongly related to the sensation of refreshment and hence most beverages such as soda or beer are usually consumed chilled. Now a days the most common way to cool a beverage is the use of ice or placing the beverage in a refrigerator. But in the unavailability of the above sources cooling a drink has become very difficult. This invention brings a potential reusable device that can be used to instantly cool a beverage without ice or a refrigerator. It is based on the combination of fundamentally two principles: Le Chatelier's Principle and Joule Thomson Effect. The device consists of a container where the reactions occurs (reaction vessel), a piston .The reaction vessel is made of a heat conducting material like aluminium or copper .The reaction vessel contains an equilibrium mixture of a gas reaction .Using the piston the pressure of the system is altered which will shift the equilibrium state in response to the Le Chatelier's principle. The user will use the piston in such a way as to push the equilibrium in the endothermic direction of the equilibrium mixture due to which temperature of the reaction vessel decreases and heat flows from the beverage to the reaction vessel to attain thermal equilibrium with it. Because of this heat flow, the temperature of the beverage cools. On expanding the reaction vessel, an additional effect of cooling occurs due to the Joule Thomson effect.

II. RELATED WORKS

If no refrigeration source is available, the beverages have to be consumed at the environmental temperature in which they are stored. Recently a number of new methods have come to cool objects. Thus, the beverages can be directly chilled without having to use a refrigeration unit. Examples include the Cooper cooler. For chilling a can it is 40 times faster than a freezer and for chilling a wine bottle it is 10 times faster than a freezer. Another type of device is the petlier cooler, cooler that uses the thermoelectric seebeck effect to cool. The third kind of coolers are the instant coolers using chemical endothermic reactions which are currently being used to create instant ice packs .They use ammonium nitrate, calcium ammonium nitrate or urea.

While these inventions may be adequate for their intended purposes, each have certain disadvantages. The Cooper cooler's the major disadvantage is that Ice is melted every time you chill a beverage. The amount of ice is the same as if you added the ice directly to the beverage. This amounts to roughly 4 typical ice cubes (25ml each) for each beverage chilled. Certain Champagne/sparkling wine bottles may not fit in the Cooper Cooler It can cool cans in 1 minute, bottles in 3.5 minutes, and wine bottles in 6 minutes. So ice is still required. On the other hand the petlier cooler cools a beverage much slower than a regular refrigerator since they are not completely sealed to allow the cold air to do its job of chilling the bottle. They use Narrow band-gap semiconductors because of room temperature operation, heavy

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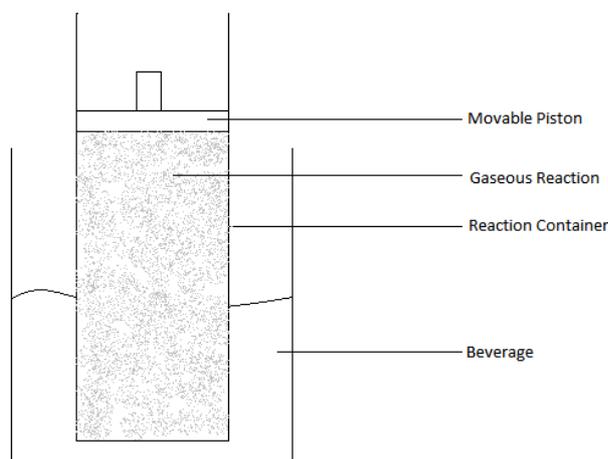
elements because of their high mobility and low thermal conductivity. Large unit cell, complex structure, highly anisotropic or highly symmetric complex compositions. Further only a limited amount of heat flux is able to be dissipated, relegated to applications with low heat flux, not as efficient, in terms of coefficient of performance, as vapour-compression systems and are much more expensive. Lastly the coolers using chemical reactions are based on chemicals which are poisonous making them dangerous. Secondly they can only be used once, making them more expensive than reusable ice packs or home-made ice packs.

Each of these disadvantages are overcome with the following invention. It is based on the Le Chatelier's principle which states that if a constraint (such as a change in pressure, temperature, or concentration of a reactant) is applied to a system in equilibrium, the equilibrium will shift as to tend to counteract the effect of the constraint. Additionally the Joule Thomson effect states that if the expansion process is reversible, meaning that the gas is in thermodynamic equilibrium at all times, it is called an isentropic expansion. In this scenario, the gas does positive work during the expansion, and its temperature decreases. Using these two principles the device can cool the beverage quickly and prevent the above disadvantages.

III. SCOPE OF RESEARCH

In the following paper the dynamic aspects of the entire cooling process has been analysed. However, a general reaction has been taken into consideration as a suitable reaction has not been found yet. Additionally the mathematical aspects in the form of equations have been used to highlight and bring out the respective requirements for the potentially possible reaction.

IV. PROPOSED METHODOLOGY AND DISCUSSION



(Drawing of Proposed Device)

As an example take an equilibrium composition of the reaction
 $2B \rightleftharpoons A$ with $-ve$ enthalpy change

Now suppose we isothermally expand it the pressure of the system will decrease. According to Le Chatelier's principle, decrease in the pressure should affect the equilibrium in such a way to increase the pressure. This implies that the equilibrium will shift in the direction which has larger number of moles of the gaseous substance. Because of this the amount of B will start increasing. Conversion of A to B is an endothermic reaction. So it will start absorbing heat from the beverage because which the temperature of beverage will start decreasing.

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The temperature of the reactants also simultaneously changes.

According to van't Hoff Equation

$$\ln\left(\frac{K_{p2}}{K_{p1}}\right) = \frac{\Delta H}{2.303R} \left(\frac{T_2 - T_1}{T_1 * T_2}\right) \quad (1)$$

As the temperature of the reaction system goes on decreasing and $-ve\Delta H$, according to the above equation, the equilibrium will again start shifting towards A.

The following equations can be used to describe the above dynamic system:



Assume we start with their concentrations of x and y respectively, and they are at equilibrium initially. The no of moles initially is also x and y as we are taking initial volume as 1 L.

Therefore

$$K_c = \frac{y^2}{x} \quad (2)$$

After doubling the volume of the reaction vessel, the concentrations of both the reactants becomes half and so

$$Q_c = 0.5 \frac{y^2}{x} \quad (3)$$

So the equilibrium shift forward and the reaction starts to proceed forward to regain equilibrium.

Let the initial concentration of A be $[A_0]$ which is $x/2$ and let the initial concentration of B be $[B_0]$ which is $y/2$.

Let the concentration of A at time t be $[A]$ and B be $[b]$ respectively. After time t the amount of $[A]$ reacted will be $[A_0]-[A]$ and so the concentration increase in B will be twice that of decrease in A according to the stoichiometry of the equation. So the amount of B after time t will be $[B_0] + 2([A_0]-[A])$.

As this is a reversible reaction the rate of change of concentration of A will be equal to rate of increase of A – rate of decrease of A. Then the rate expression is:

$$\frac{d[A]}{dt} = K_b(2[A_0] - 2[A] + [B_0]) - K_f[A] \quad (4)$$

Where

$$K_b = A_b e^{-E_{ab}/RT} \quad (5)$$

And

$$K_f = A_f e^{-E_{af}/RT} \quad (6)$$

Substituting equation 5, 6 in equation 4 and rearranging we get:

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$$\begin{aligned} \frac{d[A]}{dt} & \quad (7) \\ & = -[A] \left(2A_b e^{-\frac{E_{ab}}{RT}} + A_f e^{-\frac{E_{af}}{RT}} \right) \\ & \quad + A_b e^{-\frac{E_{ab}}{RT}} (2[A_0] + [B_0]) \end{aligned}$$

Assuming ΔH to be constant over this temperature because its variation is very less and transfer of

To be instantaneous we get the following equations.

Also According to the principles of thermodynamics the amount of heat required to change

Temperature by DT is given by

$$Q = c * dT * m \quad (8)$$

Where

c = specific heat capacity of the beverage.

And m = mass of the beverage to be cooled.

Also the heat released if α amount of B reacts is given by

$$Q = \Delta H * d[A] \quad (9)$$

Combining Equation 8 & 9 to eliminate Q we get

$$\frac{d[A]}{dT} = \frac{c * m}{\Delta H} \quad (10)$$

Solving this differential equation we get

$$[A] = \frac{c * m}{\Delta H} * T + C_1 \quad (11)$$

Substituting equation 10 and 11 in equation 7 to eliminate $[A]$ we get

$$\begin{aligned} \frac{dT}{dt} & \quad (12) \\ & = -\frac{\Delta H}{c * m} \left(\frac{c * m}{\Delta H} * T \right. \\ & \quad \left. + C_1 \right) \left(2A_b e^{-\frac{E_{ab}}{RT}} + A_f e^{-\frac{E_{af}}{RT}} \right) \\ & \quad + A_b e^{-\frac{E_{ab}}{RT}} (2[A_0] + [B_0]) \end{aligned}$$

Solving this differential equation we get

$$T = -\left(A_f e^{-\frac{E_{af}}{RT}} * A_b e^{-\frac{E_{ab}}{RT}} (2A_f C_1 e^{\frac{E_{af}}{RT}} + A_b e^{\frac{E_{ab}}{RT}} + 2A_f C_1 \frac{c * m}{\Delta H} T e^{\frac{E_{af}}{RT}} + A_b \frac{c * m}{\Delta H} T e^{\frac{E_{ab}}{RT}} - A_f e^{\frac{E_{af}}{RT}} * (2[A_0] + [B_0])) \right) / T + C_2$$

This represents Temperature, T , as a function of Time, t .

The value of initial concentrations and the value of ΔH is dependent on the maximum pressure we can apply.

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Now after the beverage has been cooled, the gas container has to be compressed again. The current volume of the container is 2L and the temperature is 30 degrees Celsius. So to get back to the initial state, two stages occur:

- 1) Instantaneous isothermal compression to 1L.
- 2) Reaction occurs backward to regain equilibrium

Now the concentration has changed and so the reaction starts moving backwards according to le Chatelier's principle.

Let the concentration of A before compression be x and that of B be y . Now we compress this 2L container instantaneously and isothermally. So the maximum pressure that can be applied by us should be greater than the pressure that $x+y$ moles of these gases exert when they are in a 1L container. Taking the maximum pressure that humans can apply as 93750Nm^{-2} and by using the ideal gas equation:

$$P * V = n * R * T \quad (13)$$

We can calculate $n = x+y = 11.276$ moles. Taking it approximately 11 moles.

Also K_c at 30 degrees Celsius can be written as:

$$K_c = 0.5 \frac{y^2}{x} \quad (14)$$

Now after compression let the 2α number of moles of B react to give α moles of A. So the final number of moles of A will be $x+\alpha$ and that of B will be $y-2\alpha$.

$$K_c = \frac{(y - 2\alpha)^2}{x + \alpha} \quad (15)$$

Again
we
can
write:

We also know that amount of heat release during this reaction will be the same as the amount of heat absorbed during expansion:

So

$$\alpha * \Delta H = c * m * \Delta T \quad (16)$$

Solving equation 14, 15, 16 and substituting $x+y = 11$, we get the following relationship between ΔH and K_c .

$$\alpha = \frac{1}{8}(-3k+4(22k+k^2)^{0.5}-(-176-7k^2-8k(22k+k^2)^{0.5}+16(22k+k^2))^{0.5} \quad (17)$$

And

$$x = n + k + (k^2 + 2nk)^{0.5} \quad (18)$$

And

$$\frac{c * m}{\Delta H} = \alpha / \Delta T \quad (19)$$

Also $2[A_0] + [B_0] = (2x + y)/2$

So we get

$$\frac{2[A_0] + [B_0]}{2} = \frac{2n + k + (k^2 + 2kn)^{0.5}}{2} \quad (20)$$

Also

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$$K_c = (A_f e^{-\frac{E_{af}}{RT}}) / (A_r e^{-\frac{E_{ar}}{RT}}) \quad (21)$$

For different requirements based on the above model we can assess the feasibility of the device and find the value of ΔH of the chemical reaction which will be suitable.

For example the beverage we want to cool is 250 ml orange juice can from 30 degrees C to 5 degrees C.

$C = 3.73 \text{ kJ kg}^{-1}\text{C}^{-1}$

And mass of the orange juice as 0.2625 kg

And $R = 8.314 \text{ J Pa K}^{-1} \text{ mol}^{-1}$

To find the value of C_1 in equation 11 the following limits can be taken:

Limits of $[A]$ is from $2(x + \alpha)$ to $[A]$ and the limits of $[B]$ is from 303K to T

And we get the value of C_1 as $-303 \frac{C \cdot m}{\Delta H} + 2(x + \alpha)$

In the function of T in t, as at time $t=0$ the temperature is 303K we get the value of C_2 as 303.

And For the reaction to be easily reversible the following condition shall be satisfied

$$10^{-3} < K_c < 10^3 \quad (22)$$

V. RESULTS

On plotting the function of temperature T vs time t we get the following results:

By numerical methods we can say that E_{af} & E_{ar} have negligible impact on the temperature vs time graph. Therefore $K = a/b$.

Keeping K_c value as 0.001 the above curve is obtained. The graph above depicts that the beverage will reach 1K in 40 seconds, and the value of ΔH is 1140 kJ. (Fig. 1, 2)

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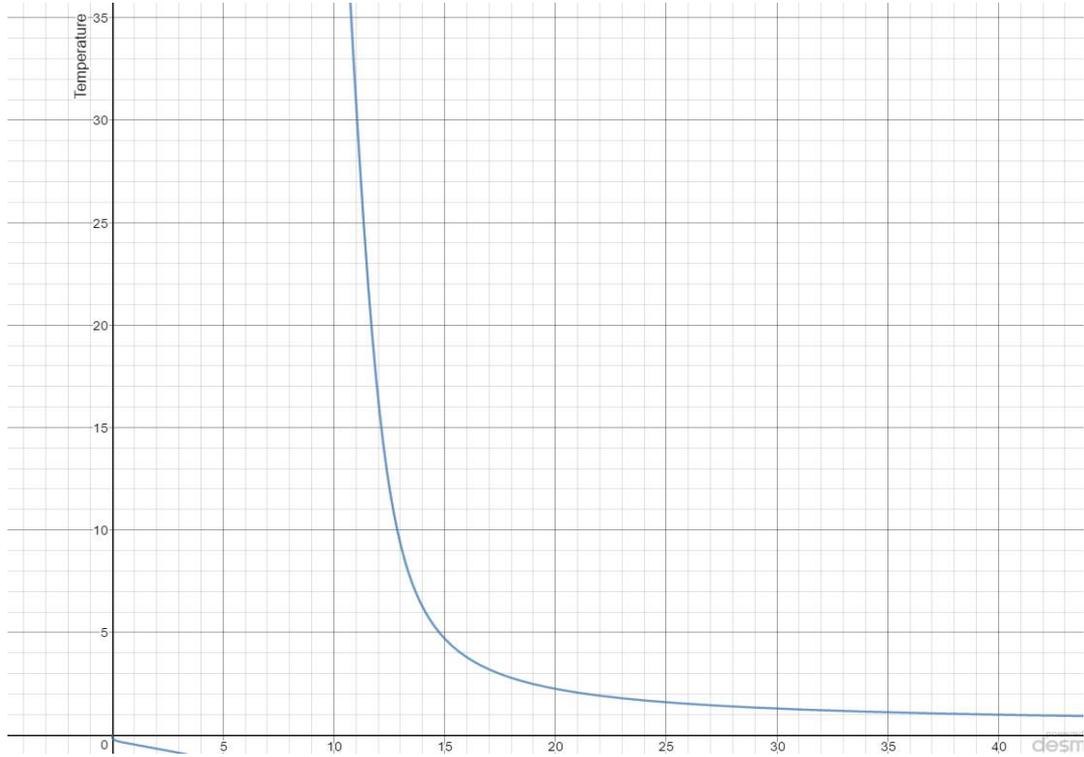


Fig.1

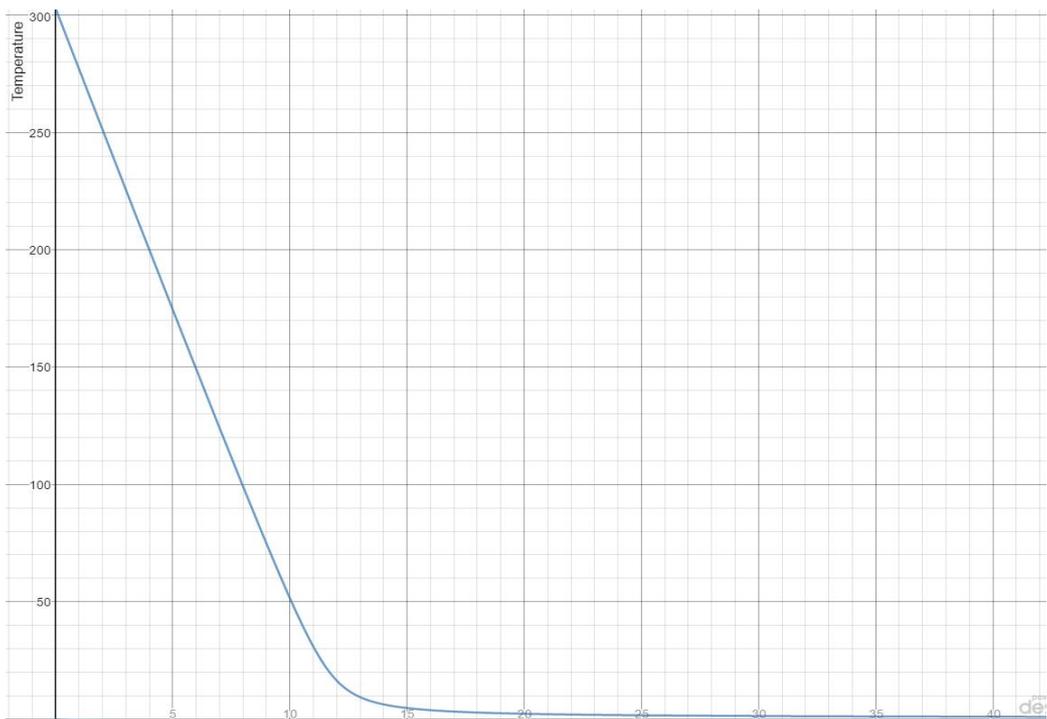


Fig 2

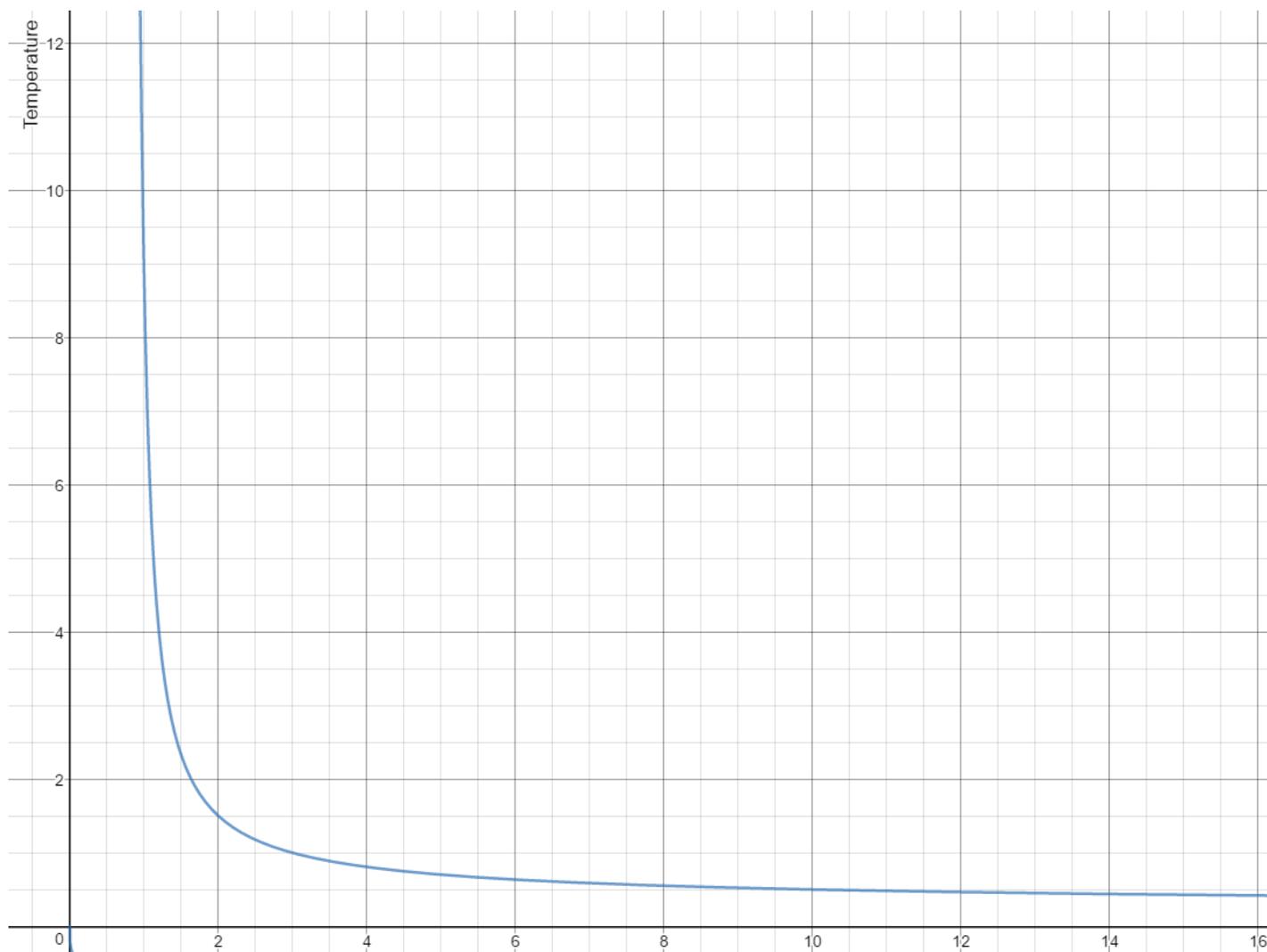


Fig 3

Keeping K_c value as 0.1 the above curve is obtained. The graph above depicts that the beverage will reach 0.5 K in 15 seconds, and the value of ΔH is 123 kJ. (Fig. 3)

Graphing for various values of K_c we find on increasing the value of K_c more cooling can be achieved in lesser time. After analysing the situation carefully the reactants of the gaseous reaction shall satisfy the following condition:

- 1) Use a Gaseous reaction: So that the reaction can stay in equilibrium and we can shift the equilibrium on changing pressure.
- 2) The K_c value should lie between 10^{-3} to 10^3 so that it can be easily reversed: So that once we can reuse it.
- 3) Spontaneous reaction after shifting the equilibrium
- 4) The boiling point of the gases should be less than 5 degrees Celsius .Because if the boiling point is more than this the gases will condense before this point itself and the concentration of the gases cannot be altered by changing the pressure if they are in the liquid state.

Note: The boiling point we are considering should be the boiling point of the gas under the high pressure we have compressed it to.

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- 5) The products and reactant should have a difference in number of moles: Changing the pressure will shift the equilibrium only if the above condition is satisfied.

VI. CONCLUSIONS

The advantages of this device is:

- 1) It does not require ice or precooling to cool the beverage which other devices like the cooper cooler requires.
- 2) It can be used to cool any beverage in any container as only the container has to be inserted .It is also much easier to transport.
- 3) It does not use highly expensive materials like Narrow band-gap semiconductors, heavy elements, and large unit cell, and complex structure, highly anisotropic or highly symmetric complex compositions.
- 4) It is reusable as the reaction vessel can be compressed again to the initial condition and can be reused again by expanding it.
- 5) The feasibility and selection of the appropriate gaseous mixture can be identified based on the calculations as illustrated above.

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BIOGRAPHY



Kshitij Gupta, is a class 12 student studying at AECS Maaruti Magnolia PU School. He has a passion for science and mathematics. He has particular interest in systems and concepts that requires interplay of Physics, Chemistry and Mathematics. He has a keen eye for problemsfaced by people in their daily lives and enjoys working on creating solutions to these problems.