

# Probability Distribution and Measure of Statistical Entropy

Selina B. Balderas and Rohitha Goonatillake \*

Texas A&M International University, Department of Mathematics and Physics, Laredo, Texas 78041-1900, USA

Received: 2 May 2021, Revised: 10 Sep. 2021, Accepted: 18 Sep. 2021

Published online: 1 Dec. 2021

**Abstract:** Enthalpy and entropy are complex concepts in thermodynamics that are not usually used in everyday life, as we do not take the time to calculate the energy needed to heat a cup of water to make tea or coffee. However, these two states are fundamental for the emergence of innovative ideas in various fields of science by improving upon existing ideas to obtain larger number of products with the maximum output of usable energy in a system. We know the modern world is characterized by high energy consumption; therefore, there are several scientists and analysts continuously investigating new methods to achieve a more efficient use of energy. In this paper, we will focus on classical and quantum physics in the subject of thermodynamics. We apply the advantages of statistical analysis to make the relationship between entropy and the number of micro-states in a system. The resulting work is microscopically characterized by a volume, energy, temperature, or number of particles that gives us a way to justify thermodynamics behavior at a microscopic level.

**Keywords:** Enthalpy, Entropy, Superconductivity, Maxwell-Boltzmann, Regression.

## 1 Introduction

The invention of the steam engine gave rise to the industrial revolution and prompted the study of heat and temperature giving rise to thermodynamics, the science that studies the movement of heat and is based on four fundamental postulates called "the four laws of thermodynamics." The zero law predicts the two bodies are in thermal equilibrium with same third body. The first is the law of conservation of energy. The second law is the entropy principle. And the third law says that there is a temperature so low that it can never be reached (absolute zero). Surely the first thing we think of when reading the word thermodynamics is heat and temperature, so it is important to be clear about the definition of these two words that are repeated frequently throughout the paper. Heat is the most common form of energy in the universe and is defined as a type of energy that is transmitted. In thermodynamics, temperature is a quantity proportional to the average kinetic energy of the molecules. That is, when something is hot it is because its molecules are moving very fast.

As we know that there exists different environments on thermodynamics, each environment contains different properties that construct our system, and the collection of

a very large number of systems is what we call an ensemble. The most important environments on the ensembles are: (a) microcanonical what is an isolated system where we have the information about the number of molecules ( $N$ ), volume ( $V$ ), and energy ( $E$ ); (b) canonical what is a close isothermal system, here the information  $N$ ,  $V$ ,  $T$  (temperature) are given; and (c) grand canonical what is an open isothermal system, where  $\mu$  = chemical potential,  $V$  and  $T$  are the information given [1]. For the moment all we need to relate, is that in the second law of thermodynamics is considered an isolated system. This second law states that the heat energy flows naturally from a hot body to a cold one but not the other way around. Also, heat cannot be transformed at 100% efficiency. This is because, in each transformation, part of the total energy is lost in the environment and loses the ability to produce changes, becoming unapproachable [2]. Because heat is an isolated system; over time, the disorder increases. In physics, this disorder is known as Entropy ( $S$ ), and it measures the amount of energy that is dissipated in continuous transformations and cannot be recovered. On the other hand, enthalpy ( $H$ ) defined the total amount of energy that a system contains and is used to measure the energy variations that occur, either when taking or releasing

\* Corresponding author e-mail: [harag@tamiu.edu](mailto:harag@tamiu.edu)

energy into the environment. Enthalpy and entropy are related through temperature, a relationship that is reflected in the equation (1):

$$T\Delta S = \Delta H, \quad (1)$$

where  $T$  is the absolute temperature,  $\Delta H$  is the change in enthalpy, and  $\Delta S$  is the change in entropy. As can be deduced from the equation, if the temperature is kept constant, an increase in enthalpy causes an increase in its entropy, and vice versa. The minimum value of entropy is reached at  $-273.15^\circ\text{C} = 0^\circ\text{K}$ , also known as absolute zero. The closer the temperature is to this absolute zero, the molecules do not move or react, but when we incorporated heat into the system the molecules will begin to react causing an increase in disorder (collide with each other), exchanging kinetic energy. The higher the temperature, the higher these kinds of interactions (collisions) will be and the molecules will travel faster. We already know we can not use 100% efficiency of the energy in a system, now we have the question. How many energy we can use? Free energy, also known as Gibbs free energy ( $G$ ), is a measure of the amount of energy usable to do work in a system. The change in Gibbs free energy during a reaction provides useful information about the energy and spontaneity of the reaction. This value indicates the maximum usable energy released or absorbed when going from the initial state to the final state. Furthermore, its sign (either positive or negative) tells us whether a reaction will occur without additional energy. The free energy ( $\Delta G$ ) is given by:

$$\Delta G = \Delta H - T\Delta S, \quad (2)$$

the change in enthalpy ( $\Delta H$ ), change in entropy ( $\Delta S$ ), and temperature ( $T$ ). A given temperature along a path that provides free energy corresponds to the marginal likelihood and/or Bayes factor where the distribution with maximal information entropy is the best choice [3]. As we are going to find a different statistical probability distributions for the purpose of this paper, the Maxwell-Boltzmann speed distribution tells us the probability of finding an atom or molecule in the gas with any particular speed. We can use this information to make powerful statements about the Gaussian system as a whole by computing average properties from the probability distribution [4]. There are different states of matter, and in each one the particles will have different behaviors when the heat increases. Solid, liquid and gas are not the only states of aggregation of matter. There is also the plasma as the fourth state. And there are even others like the Bose-Einstein condensate, the Fermi condensate, the supersolid, and the quark-gluon plasma. If we do not know them, it is because they do not occur naturally in the environment. We will see later when a Bose-Einstein condensate reaches the smallest possible value of entropy at the absolute zero the superconductivity emerges. Superconductivity is the phenomenon that occurs in some substances in which

their electrical resistance disappears when the temperature is reduced below a critical point temperature (close to the absolute zero). At this temperature the magnetic field inside a superconductor is zero and the magnetic induction is expelled from the interior. This situation is called the Meissner effect and it is verified by levitating a magnet on the superconductor immersed in liquid Nitrogen.

At these temperatures, the particles cease to be separate elements and work as a single atom. The most fascinating thing is that this field of thermodynamic research continues open to new ideas, not only in the area of physics, also for analytical chemistry, statistics, biophysics and much more. The use of calorimetry and thermodynamics helps in design and discover new drugs for human beings. As Lowe [5] writes in his article "Enthalpy and Entropy Again" and Chaires [6] in his article "Calorimetry and Thermodynamics in Drug Design" they are modern theories, recently discussed around 2008. Both, Lowe (2010) and Chaires (2008), propose that the use of modern instrumentation for calorimetry permits direct determination of enthalpy values for binding reactions and conformational transitions in biomolecules. The free energy, enthalpy, and entropy are of enormous value in drug design because they provide information about the balance of driving forces that cannot be obtained from structural or computational methods alone.

## 2 Methodology

### 2.1 Statistic Entropy

Entropy and the second law of thermodynamics have a statistical interpretation in a variation of calculus applied to probability distributions. We have already learned at the beginning that the entropy measures the amount of energy that is dissipated in continuous transformations and cannot be recovered. The entropy is denoted by  $S$ , and is given by:

$$S = -K_B \sum_i p_i \ln p_i \quad (3)$$

or

$$S = K_B \ln \Omega, \quad (4)$$

where  $\Omega$  is the number of micro-states consistent with the macro-state, for  $\Omega \in \mathbb{N}$  and  $S \geq 0$  ( $\ln(1) = 0$ ,  $\ln \Omega \geq 0$ ). In an easier way,  $\Omega$  is the number of micro-states, and natural logarithm is used to have an easier expression of the numbers of macro-states that give rise to the micro-state that make up the entropy. But what makes  $-K_B \sum_i p_i \ln p_i$  different from  $K_B \ln \Omega$ ? The first one is the Gibbs definition, where he tried to find the probability of choosing among all the possibilities the micro-state  $i$ , that creates this entropy, this probability being given by  $p_i$ . And the second  $K_B \ln \Omega$  is the entropy of Boltzmann,

where both (Gibbs and Boltzmann entropy) are exactly the same expression. Therefore, the entropy is just a number of which the more the numbers of microscopic states given by a macro-state increase, the probability will increase. In order to find the change in entropy of a real process (that process that cannot be reversible) we begin in a state of system A and end in the state of system B. finding:

$$\Delta S = \int_A^B \frac{dQ}{T}. \quad (5)$$

In an isolated system in which the energy is constant, a state of thermodynamic equilibrium is attained when the entropy is maximal [7]. According to the book of "Rational Extended Thermodynamics Beyond the Monatomic Gas" [8], the maximum of entropy (as the name says and according to the definition of entropy) is the state of a physical system at greatest disorder (in terms of statistics), or a statistical model of least encoded information.

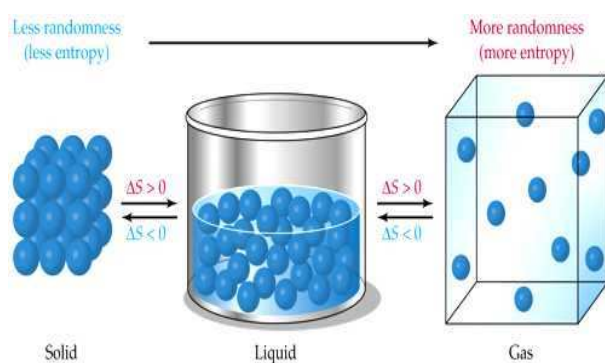


Figure 1. Three Status of Matter: Solid, Liquid, and Gas.

Source: Significance of Entropy QR Study.

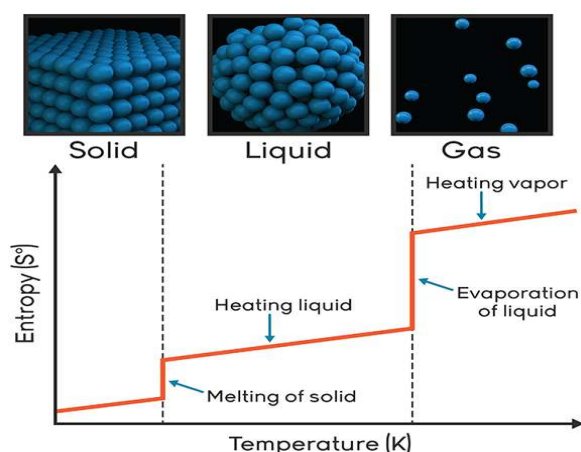


Figure 2. Relation of Entropy (S) vs Temperature (K).

Source: Annenberg Learner, Equilibrium and Advanced Thermodynamics: Balance in Chemical Reactions, 2019 [9].

In Figure 1, we can see the behavior of the particles in the solid, liquid and gas states. In Figure 2, we see that an increase in entropy is related to an increase in temperature [10]. In terms of statistics, maximum entropy has important features. As it describes, this principle states that the probability distribution which best represents the current state of knowledge is the one with largest entropy, in the context of precisely stated prior data. Ruggeri and Sugiyama (2015) give another way of stating this as: "to take precisely stated prior data or testable information about a probability distribution function. Let us consider the set of all trial probability distributions that would encode the prior data. According to this principle, the distribution with maximal information entropy is the best choice, because the distribution with the maximum entropy is the one that makes the fewest assumptions about the true distribution of data" [11].

### 2.1.1 Maximum Entropy Probability Distribution

Since we have just been introduced to the principle of maximum entropy, the distribution with the highest entropy should be chosen as the least informative default distribution. According to Jizba and Korb from Cornell University, "the motivation is two-fold. Firstly, maximizing entropy minimizes the amount of prior information incorporated into the distribution; secondly, many physical systems tend to move toward maximum entropy configurations over time [12]".

If  $X$  is a discrete random variable with distribution given by:

$$Pr(X = x_k) = p_k \quad (6)$$

for  $k = 1, 2, \dots$ , then the entropy of  $X$  is defined as:

$$H(x) = - \sum_{k \geq 1} p_k \log p_k. \quad (7)$$

If  $X$  is a continuous random variable with probability density function  $p(x)$ , then the differential entropy of  $X$  is defined as:

$$H(x) = - \int_{-\infty}^{\infty} p(x) \log p(x) dx, \quad (8)$$

where quantity  $p(x) \log p(x)$  is understood to be zero whenever  $p(x) = 0$  [12]. We know that standard deviation represents the level of dispersion of a distribution. A distribution with high standard deviation requires many bits of information to be defined, therefore we can say its entropy level is high. Entropy and standard deviation are not the same, but entropy in most cases depends on the standard deviation of the distribution.

### 2.2 Maxwell-Boltzmann Statistics

Speaking from a probability point of view, for a physical problem, an ideal gas that has an immense number of

particles, from the molecular theory of gases, it is easier and more possible for us to find these statistical features of the movement of particles. Either its distribution or partition in statistical features such as the entropy on the second law of thermodynamics, to understand the Maxwell-Boltzmann distribution it is required some knowledge about combinatorics that a total of  $N$  particles or molecules can be ordered exactly  $N! = 1 \cdot 2 \cdot \dots \cdot N$  different ways:

$$\binom{N}{n} = \frac{N!}{(N-n)!n!}, \quad (9)$$

where the equation (9) are the combinations of  $N$  elements taken from  $n = 0, 1, 2, \dots, N$ , where  $0! = 1$  for  $n = 0$ . It corresponds to the most probable energy distribution and provides the best approximation of the conditions in gas. There are different class of statistic. First is the classical statistic (Maxwell-Boltzmann), and second, the quantum statistic (Bose-Einstein and Fermi-Dirac statistics). The parameters used for the classical or Maxwell-Boltzmann statistics, are given below [13].

Table 1. Parameter for Maxwell-Boltzmann Statistic.

| STATISTIC                              |                                                                                                                                                          |
|----------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|
| Parameter                              | Maxwell-Boltzmann.                                                                                                                                       |
| Particles                              | Particles are distinguishable.                                                                                                                           |
| Size of phase space cell               | The size of phase space cell can be as small as we require.                                                                                              |
| Number of cells                        | If $n_i$ be the number of particles and $g_i$ the number of cells then $g_i \gg n_i/g_i \ll 1$ . Thus, number of cells can be made as large as possible. |
| Restriction on particles               | No restriction.                                                                                                                                          |
| Two particle distribution in two cells | The particles are distinguishable and can be arranged in four ways: $(A B), (B A), (AB ), ( AB)$ .                                                       |

With the parameters of the Maxwell-Boltzmann statistic, given our Gaussian system, we can divide our system as many sufficiently small cells as needed as seen in Table 1. The Maxwell and Boltzmann tells us that we can predict in which cells the particles or molecules of the system are going to end. If we take molecules of water, for example, there are  $6.022 \times 10^{23}$  molecules of water per mole. If we tried to predict by hand all the possible combinations of all these molecules in all the cells given to the system, it would take us more than a trillion years to achieve all the possible combinations. For example, suppose that in a system of  $N$  distinguishable and independent particles with total energy  $E = 6\epsilon$ , the available energy levels for each particle is  $\epsilon_j = j\epsilon$ , for  $j = 0, 1, 2, \dots, i$ . All possible macrostates and their probabilities in our example where  $N = 20$  simple random samples is given in Table 2.

Table 2. Distribution and Probability of 20 Simple Random Samples.

| Dist. | 0  | $\epsilon$ | $2\epsilon$ | $3\epsilon$ | $4\epsilon$ | $5\epsilon$ | $6\epsilon$ | Micro-states | Probability            |
|-------|----|------------|-------------|-------------|-------------|-------------|-------------|--------------|------------------------|
| 1     | 19 | 0          | 0           | 0           | 0           | 0           | 1           | 20           | $1.129 \times 10^{-4}$ |
| 2     | 18 | 1          | 0           | 0           | 0           | 1           | 0           | 380          | $2.146 \times 10^{-3}$ |
| 3     | 17 | 2          | 0           | 0           | 1           | 0           | 0           | 3,420        | $1.931 \times 10^{-1}$ |
| 4     | 18 | 0          | 1           | 0           | 1           | 0           | 0           | 380          | $2.146 \times 10^{-3}$ |
| 5     | 17 | 1          | 1           | 1           | 0           | 0           | 0           | 6,840        | $3.659 \times 10^{-1}$ |
| 6     | 18 | 0          | 0           | 2           | 0           | 0           | 0           | 190          | $1.073 \times 10^{-3}$ |
| 7     | 16 | 3          | 0           | 1           | 0           | 0           | 0           | 19,380       | $1.094 \times 10^{-1}$ |
| 8     | 17 | 0          | 3           | 0           | 0           | 0           | 0           | 1,140        | $6.437 \times 10^{-3}$ |
| 9     | 16 | 2          | 2           | 0           | 0           | 0           | 0           | 29,070       | $1.641 \times 10^{-1}$ |
| 10    | 15 | 4          | 1           | 0           | 0           | 0           | 0           | 77,520       | $4.377 \times 10^{-1}$ |
| 11    | 14 | 6          | 0           | 0           | 0           | 0           | 0           | 38,760       | $2.189 \times 10^{-1}$ |

For a configuration of  $n_1, n_2, \dots, n_p = n_i$  particles with energy  $\epsilon_i$ , working with an isolated gas implies that the number of particles  $N$  and the sum of the energies  $U$  are fixed, which is called total internal energy. This gives the possibility that the particles are distributed in the following energy levels:

$$\frac{N!}{\prod_i n_i!} \text{ for } \begin{cases} N = \sum_i n_i, \\ U = \sum_i n_i \epsilon_i. \end{cases} \quad (10)$$

The first distribution is where one particle is in the cell  $6\epsilon$  and the 19 remainder in the cell  $0\epsilon$ . In this example,  $N! = 20!$ , and  $\prod_i n_i! = 19! 1!$ . Therefore,  $\frac{N!}{\prod_i n_i!} = \frac{20!}{19! 1!} = 20$ . The second distribution is where 18 particles are in the cell  $0\epsilon$ , one in  $\epsilon$ , and one in  $5\epsilon$ ; thus  $\frac{N!}{\prod_i n_i!} = \frac{20!}{18! 1! 1!} = 380$ . As we see in Table 2, there are 177,100 different ways to arrange just 20 simple random samples in  $6\epsilon$ . If we change the energy to  $12\epsilon$ , the total number of different ways to arrange these 20 samples should greatly increase, even more so if we consider a bigger number of particles. Now we consider all the possible combinations in a Gaussian system where particles tends to infinity. To be able to study the distribution most likely to be generated, it is necessary to know when the maximum likelihood estimation reached with (10) [14], where it is easier to work with the natural logarithm as:

$$\log(n!) = \log 2 + \log 3 + \dots + \log n. \quad (11)$$

In this way, we need to calculate the maximum of the next mathematic expression

$$F(x_1, x_2, x_3, \dots) = N \log N - N - \sum_i (x_i \log x_i - x_i), \quad (12)$$

where  $x_i \geq 0$ , conditional on the amounts of  $N$  and  $U$  which are fixed. By means of the Lagrange multipliers we will denote  $\alpha$  and  $\beta$  as the multiplier parameters of the underlying context:

$$-\log x_i - \alpha \cdot 1 - \beta \varepsilon_i = 0. \quad (13)$$

As a result,  $x_i = \exp^{-\alpha - \beta \varepsilon_i}$  and by retrieving the initial numbers  $n_i \iff x_i$  and imposing  $N = \sum_i n_i$  we get:

$$n_i = \frac{N}{Z} \exp^{-\beta \varepsilon_i}, \quad (14)$$

where we can define  $Z$  as:

$$Z = \sum_i \exp^{-\beta \varepsilon_i} \text{ or } Z = \sum_i g_i \exp^{-\varepsilon_i / K_B T}, \quad (15)$$

where  $Z$  is called the partition function, and this constant gives us the normalization for a total number of particles be equal to  $N$ . In the Maxwell-Boltzmann distribution explanation we will give more focus on why  $\beta = \frac{1}{K_B T}$ , where  $K_B$  = Boltzmann constant,  $T$  is the absolute temperature and  $g_i$  is the degeneracy of energy lever  $i$ . But for the moment we will leave it like that. In this way, and usually in many books, the expected number of particles with energy  $\varepsilon_i$  is given by:

$$\langle N_i \rangle = \frac{g_i}{\exp(\varepsilon_i - \mu) / K_B T} = \frac{N}{Z} g_i \exp^{-\varepsilon_i / K_B T}. \quad (16)$$

Something similar to this we already have as follows:  $\varepsilon_i = i^{th}$  energy level,  $g_i$  is the degeneracy (when two or more quantum mechanical system have the same value of energy upon measurement) of energy lever  $i$ ;  $\mu$  is the chemical potential (energy can be absorbed);  $K_B$  = Boltzmann constant =  $k_b = 1.38064852(79) \times 10^{-23} \text{ J/K}$  or  $1.38064852 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$ ;  $T$  is the absolute temperature;  $N$  is the total number of particles  $N = \sum_i N_i$ ;  $Z$  is the partition function  $Z = \sum_i g_i \exp^{-\varepsilon_i / K_B T}$ .

### 2.2.1 Maxwell-Boltzmann Distribution

According to the Maxwell-Boltzmann statistic the probability that a system of these particles with mass  $m$ , one of them has a velocity  $v$  between  $v_0$  and  $v_0 + \Delta$  for a small but  $\Delta > 0$  is given by:

$$P(v_0 < v < v_0 + \Delta) \approx K \Delta \exp^{-\frac{1}{2} \beta m v_0^2} \text{ as } \Delta \rightarrow 0, \quad (17)$$

the velocity of each particle is given by three coordinates  $v = (v_x, v_y, v_z)$ . Using the previous formula in each

coordinate the probability that a particle has the end of its velocity vector is approximately,

$$K^3 \Delta^3 \exp^{-\frac{1}{2} \beta m (v_x^2 + v_y^2 + v_z^2)}. \quad (18)$$

For a spherical crown volume,  $R < (X^2 + Y^2 + Z^2)^{1/2} < R + \delta$  with a really small value for  $\delta > 0$ , the volume approach to  $4\pi R^2 \delta$ , the area of the spherical surface times the thickness. Consequently, if we take cubes of the side  $\Delta$  more smallest than  $\delta$ , can be fit in  $4\pi R^2 \delta / \Delta^3$  with better approximation when  $\Delta$  decreases. Therefore, the probability that the velocity  $(v_x^2 + v_y^2 + v_z^2)^{1/2}$  can be between  $v$  and  $v + \delta$  is  $K' \delta v^2 \exp^{-\frac{1}{2} \beta m v^2}$ . For a really small value of  $\delta$ , the sum gives us the following integration as  $\delta \rightarrow 0$ :

$$K' \int_0^\infty v^2 \exp^{-\frac{1}{2} \beta m v^2} dv = 1. \quad (19)$$

Therefore, the probability that a particle in a gas has a velocity given by:

$$\delta \sqrt{\frac{2}{\pi}} (\beta m)^{\frac{3}{2}} v^2 \exp^{-\frac{1}{2} \beta m v^2}. \quad (20)$$

We now consider the variable  $X = \sqrt{X_1^2 + X_2^2 + X_3^2}$  with  $X_i$ 's independents and distributed according  $N(0, \sigma)$  with  $\sigma = 1/\sqrt{m\beta}$ . Here  $X/\sigma$  follows a distribution  $X$  with three degrees of freedom, with density function  $g(x) = \sqrt{2/\pi} x^2 \exp^{-x^2/2}$ , and the density function for  $X$  is  $\sigma^{-1} g(x/\sigma)$  what correspond to Maxwell-Boltzmann distribution. We find different representation for the function and distribution as

$$f(c) = 4\pi \left( \frac{M}{2\pi K_B T} \right)^{\frac{3}{2}} c^2 \exp^{-\frac{Mv^2}{2K_B T}}, \quad (21)$$

where the probability in a graph looks as Figure 3.

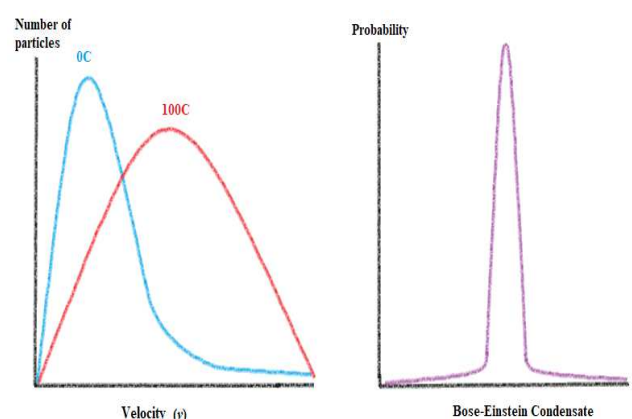


Figure 3. Maxwells' Speed Distribution.

In Figure 3, we see that the Maxwell-Boltzmann distribution is shifted to higher speeds and is broadened at higher temperatures as the dependence of the Maxwell-Boltzmann distribution on molecule mass. On average, the heavier molecules move more slowly than lighter molecules. We can have different physical interpretation of  $\beta$  as  $\beta = ZP$  [15]. Normally the value of  $\beta$  is given, but it can be obtained according to the perfect gas equation,

$$PV = nRT, \quad (22)$$

where  $P$  = pressure,  $V$  = volume,  $n$  = amount of substance,  $R$  = ideal gas constant, and  $T$  = temperature.

In other words, we can express the Maxwell distribution as the  $\mathcal{X}^2$  distribution with three degrees of freedom  $\mathcal{X}_3^2$  (components of velocity in Euclidean space  $P(x(t), y(t), z(t))$ ) as they were both follows a standard normal distribution [16].

### 3 Problems and Data

#### 3.1 Classic Physics

##### 3.1.1 Model Selection and Criticism

The validity of the assumption must be made before any conclusion are drawn from the analysis. We know that heat is a class of energy, it is related to the speed of the particles in the system. There is no limit to heat, the faster the particles move the more heat the system will have. For this experiment, it is logical to assume that enthalpy and entropy are related to temperature. We are going to show that both enthalpy and entropy are dependent from temperature and from each other ( $H$  and  $S$  are dependent events, and dependent for  $T$ ). Once we show the first assumptions of dependence and independence, then we will assume and show that there is going to be a strong positive relation between temperature vs. enthalpy, temperature vs. entropy, and enthalpy vs. entropy. Letting  $H$  and  $S$  are dependents to each other and with  $T$ , we can predict future behaviors with these two values.

A cross-over design is usually used for clinical advancements, but for this study, it will only be used to create random blocks.  $SH$  will be assigned to the entropy vs. enthalpy difference, and  $HS$  will be assigned for the enthalpy vs. entropy difference, both with respect to temperatures.

##### 3.1.2 Experimental Process

There are different states of matter, and in each one, the particles will have different behaviors when the energy increases. We know that water can be transformed into three different states according to temperature: solid, liquid and gas. The purpose of this experiment is to find the entropy and enthalpy of water (in different states) in

different temperatures, as in Figure 2. For procedure, we need to clarify the thermodynamics properties of water and the SI units associated with them as follows for clarity.

- Boiling temperature (at 101.325 kPa):  $99.974^\circ\text{C} = 211.953^\circ\text{F}$
- Bulk modulus elasticity:  $2.15 \times 10^9 \text{ Pa}$  or  $N/m^2$
- Critical temperature:  $373.946^\circ\text{C} = 705.103^\circ\text{F}$
- Critical pressure:  $217.7 \text{ atm} = 220.6 \text{ bar} = 22.06 \text{ MPa}$  ( $NM/m^2$ ) =  $3200 \text{ psi}$  ( $lb_f/in^2$ )
- Critical density:  $0.322 \text{ g/cm}^3 = 0.62478 \text{ slug/ft}^3 = 20.1018 \text{ lb}_m/\text{ft}^3$
- Ionization constant:  $pK_w$  (at  $25^\circ\text{C}$ ): 13.995
- Latent heat of melting:  $334 \text{ kJ/kg} = 144 \text{ Btu(IT)/lb}$
- Latent heat of evaporation (at  $100^\circ\text{C}$ ):  $40.657 \text{ kJ/mol} = 2256 \text{ kJ/kg} = 970 \text{ Btu(IT)/lb}$
- Maximum density (at  $4^\circ\text{C}$ ):  $999.975 \text{ kg/m}^3 = 1.9403 \text{ slug/ft}^3 = 8.34519 \text{ lb}_m/\text{gal}(US)$
- Melting temperature (at 101.325 kPa):  $0^\circ\text{C} = 32^\circ\text{F}$
- Molar Mass:  $18.01527 \text{ g/mol}$
- pH (at  $25^\circ\text{C}$ ): 6.9976

The water reach the critical point at  $374^\circ\text{C}$  ( $705.2^\circ\text{F}$ ). Therefore, we choose different temperature from  $0^\circ\text{C}$  ( $32^\circ\text{F}$ ) to  $373.946^\circ\text{C}$  ( $711.956^\circ\text{F}$ ).

The SI units are going to be Joule per mole kelvin  $J/kmol$ , and the energy per unit mass (specific energy - mass), british thermal unit (international table)/pound  $[Btu(IT)/lb]$ , gigajoule/tonne  $[GJ/t]$ , kilocalorie/kilogram  $[kcal/kg]$  = calorie/gram  $[cal/g]$ , kilojoule/kilogram  $[kJ/kg]$  = joule/gram  $[J/g]$ , kilowatt hour/kilogram  $[kWh/kg]$

- $1 \text{ Btu(IT)/lb} = 0.002326 \text{ GJ/t} = 2.326 \text{ kJ/kg} = 0.5559 \text{ kcal/kg} = 0.000646 \text{ kWh/kg}$
- $1 \text{ cal/g} = 1 \text{ kcal/kg} = 0.0041868 \text{ GJ/t} = 4.1868 \text{ kJ/kg} = 1.8 \text{ Btu(IT)/lb} = 0.001162 \text{ kWh/kg}$
- $1 \text{ GJ/t} = 1000 \text{ kJ/kg} = 429.923 \text{ Btu(IT)/lb} = 238.846 \text{ kcal/kg} = 0.278 \text{ kWh/kg}$
- $1 \text{ J/g} = 1 \text{ kJ/kg} = 10^{-3} \text{ GJ/t} = 0.23885 \text{ kcal/kg} = 0.4299 \text{ Btu(IT)/lb} = 0.0002778 \text{ kWh/kg}$
- $1 \text{ kcal/kg} = 1 \text{ cal/g} = 0.0041868 \text{ GJ/t} = 4.1868 \text{ kJ/kg} = 1.8 \text{ Btu(IT)/lb} = 0.001162 \text{ kWh/kg}$
- $1 \text{ kJ/kg} = 1 \text{ J/g} = 10^{-3} \text{ GJ/t} = 0.23885 \text{ kcal/kg} = 0.4299 \text{ Btu(IT)/lb} = 0.0002778 \text{ kWh/kg}$
- $1 \text{ kWh/kg} = 1547.7 \text{ Btu(IT)/lb} = 3.597 \text{ GJ/t} = 3,597.1 \text{ kJ/kg} = 860.421 \text{ kcal/kg}$ . [17].

#### 3.2 Quantum Physics

We introduce an experimental observation of some phenomena in the Bose-Einstein Condensates (BEC). The BEC is a state of aggregation of matter, formed by supercooled bosons close to absolute zero, in which a good part of them occupy the lowest possible quantum state. The study of the atom in superconductivity, is

essentially the particles are required to have very little movement, which will bring the Bose-Einstein condensate to temperatures that are virtually absolute zero. Another experiment that is recognized with this study is when cold atoms and Bose-Einstein condensates run across an optical dipole potential and experience parametric excitations in a quadrupole-Ioffe-configuration (QUIC) trap [18]. China has developed the first chip-based Bose-Einstein condensates for the precise use and manipulation of cold atoms.

The process consist of a double magnetic-optical trap (MOT) configuration that is employed to produce cold atoms and Bose-Einstein condensates. Two chambers are separated by 56 cm and are connected through a 28-cm-long and 3-cm-wide vertical tube. There is a 1.6 mm diameter hole in the center of the quarter wave plate with high-reflection coating. A QUIC trap is composed of a pair of quadrupole coils and an Ioffe coil to form a magnetic field without zero point. There are several processes from MOT loading to a QUIC trap [18], that included compressed MOT, polarization gradient cooling, optical pumping, quadrupole trap compression, and magnetic trapping transferring.

Table 3. Timing Process for Producing a BEC.

|                        | Atom number                   | Temperature | Time       |
|------------------------|-------------------------------|-------------|------------|
| Low MTO loading        | $6 \times 10^8$               | $300\mu K$  | 50s        |
| Compressed MOT         | $3 \times 10^8$               | $300\mu K$  | 2ms        |
| Sisyphus cooling       | $3 \times 10^8$               | $20\mu K$   | 8ms        |
| State preparation      | $3 \times 10^8$               | $20\mu K$   | 50 $\mu s$ |
| Magnetic trap loading  | $2 \times 10^8$               | $300\mu K$  | 1s         |
| QUIC trap transferring | $7 \times 10^7$               | $300\mu K$  | 0.5s       |
| Evaporative cooling    | $2 \times 10^5$<br>(pure BEC) | 200nK       | 28s        |

Source: Bose-Einstein Condensates: Theory, Characteristics, and Current Research [18].

As we learn from Table 1 with the parameters of Maxwell-Boltzmann statistic given the Gaussian system, we can divide the system into cells at any amount or size required. "One can immediately see that the entropy has to vanish at absolute zero. In fact, in this case, the molecules fall (all) into the first cell (the cell with the lowest energy); for this state there is only a single distribution of molecules according to the count." [19] This was the theoretical prediction made by Bose in 1925 that had to wait 75 years in getting confirmed experimentally as shown in Figure 19 [20].

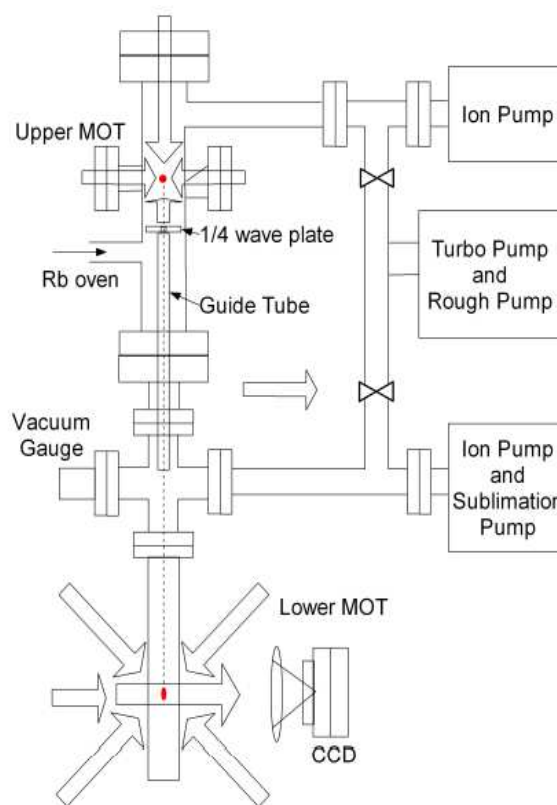


Figure 4. The QUIC Trap.

Source: Matthews, Paige E (2010). "Bose-Einstein Condensates: Theory, Characteristics, and Current Research [18]."

The timing process is listed in Table 3 and Figure 4. The latter is the machine that make the experiment possible.

## 4 Results from Classic Physics and Quantum Physics

In the following, we provide a summary of the statistical tests that have been used and the results obtained from the analyses conducted for the comparisons of the classic Physics and quantum Physics in terms of Enthalpy ( $H$ ), Entropy ( $S$ ) together with temperatures ( $T$ ).

### 4.1 Classic Physics

First, the block randomness for  $HS$  and  $SH$  are carried out at different temperatures using the statistical analysis of cross-over trial data using Satterthwaite approximation. The chief distinction is that the Satterthwaite approximation does not assume equal variances, whereas the pooled method does. We can always use the Satterthwaite method to be correct, but we only use the pooled method in very specific situation to conclude that there is significance difference between  $HS$  and  $SH$ .

In separate tests, we plotted non-parametric and parametric results for the sequences of  $HS$  and  $SH$ . A Chi-square test of significance is essentially concerned with only observed frequencies with the distinction between expected and observed frequencies, the distinction between two interval level variables, and the distinction between one ordinal and one interval level variable to see dependence or independence for  $T$  vs.  $H$  and  $T$  vs.  $S$ . It is seen that when the temperature increases with both  $H$  and  $S$  increase. There is a strong positive correlation in between the variables. As for the distributions of  $S$  and  $H$ ,  $S$  is slightly skewed to the right and whereas  $H$  approximately follows a pattern of the normal distribution. The contour fitting for temperature for known band  $S$  and  $H$  were obtained at 100°C, 200°C, and 300°C.

The REG procedure is a regression procedure in the SAS System. It is a procedure for regression, while other SAS regression procedures provide more specialized applications as we have done with dependent variables in this section. The linear regressions carried out for Entropy with temperatures and Enthalpy with temperatures concluded that Entropy can be expressed as Entropy =  $87.67 \times \text{Temperature} - 988.68$  and Enthalpy =  $0.192 \times \text{Temperature} + 2.816$  in terms of linear functions of temperature with a strong correlation in water at 20°C.

Since the water reached the critical point at 374°C (705.2°F), at this temperature, the water already transformed into a gas and will be impossible to liquefy by compression regardless of the pressure applied, making it impossible to condense. Therefore, we choose different temperature from 0°C (32°F) to 373.946°C (211.956°F) for the first part of the analysis.

Table 4. Measures of Enthalpy ( $H$ ) and Entropy ( $S$ ) at Different Temperatures.

| Temperature<br>[°C] | Enthalpy, H<br>[kJ/kmol] | Entropy, S<br>[kJ/(kmol K)] | Temperature<br>[°C] | Enthalpy, H<br>[kJ/kmol] | Entropy, S<br>[kJ/(kmol K)] |
|---------------------|--------------------------|-----------------------------|---------------------|--------------------------|-----------------------------|
| 0.01                | 0                        | 0                           | 140                 | 10614                    | 31.33                       |
| 10                  | 757.1                    | 2.722                       | 160                 | 12169                    | 35                          |
| 20                  | 1511.8                   | 5.341                       | 180                 | 13747                    | 38.54                       |
| 25                  | 1888.6                   | 6.616                       | 200                 | 15354                    | 41.99                       |
| 30                  | 2265.2                   | 7.868                       | 220                 | 17000                    | 45.68                       |
| 40                  | 3018.2                   | 10.31                       | 240                 | 18693                    | 48.68                       |
| 50                  | 3771.5                   | 12.68                       | 260                 | 20448                    | 51.97                       |
| 60                  | 4525.3                   | 14.98                       | 280                 | 22284                    | 55.28                       |
| 70                  | 5279.9                   | 17.21                       | 300                 | 24232                    | 58.65                       |
| 80                  | 6035.5                   | 19.38                       | 320                 | 26343                    | 62.14                       |
| 90                  | 6792.8                   | 21.49                       | 340                 | 28727                    | 65.94                       |
| 100                 | 7551.8                   | 23.55                       | 360                 | 31739                    | 70.56                       |
| 110                 | 8312.9                   | 25.56                       | 373.946             | 37551                    | 79.4                        |
| 120                 | 9076.6                   | 27.53                       |                     |                          |                             |

Source: Engineering ToolBox, (2009) [21].

According to the statistical analysis of cross-over trial data, both carryout effects  $\mu_{HS} = \mu_{SH}$ . This implies that when we compare the two sequences with respect to their differences  $\mu_{HS} - \mu_{SH} = 0$  that make no difference for both sequences in period 1 and period 2. If the null hypothesis,  $H_0 =$  no difference and  $H_1 =$  two treatments, then they are significantly different. If we end with  $p\text{-value} \leq 0.05$ , then we reject the null hypothesis  $H_0$ , meaning both are significantly different.

```

data values;
samplesize=27;
blocksize=3;
run;
data random;
set values;
nblocks=round(samplesize/blocksize);
na=round(blocksize/2);
nb=blocksize-na;
do block=1 to nblocks by 1;
  nna=0;
  nnb=0;
  do i=1 to blocksize;
    subject=i+((block-1)*blocksize);
    if nna=na then treatment="HS";
    if nnb=nb then treatment="SH";
    else do;
      aprob=(na-nna)/(na+nb-nna-nnb);
      u=ranuni(0);
      if (0<=u<=aprob) then do;
        treatment="SH";
        nna=nna+1;
      end;
      if (aprob<u<1) then do;
        treatment="HS";
        nnb=nnb+1;
      end;
    end;
  end;
  keep subject treatment;
  output;
end;
run;

proc print data=random;
id subject;
var treatment;
run;

```

| subject | treatment |
|---------|-----------|
| 1       | SH        |
| 2       | HS        |
| 3       | SH        |
| 4       | SH        |
| 5       | HS        |
| 6       | SH        |
| 7       | SH        |
| 8       | SH        |
| 9       | HS        |
| 10      | SH        |
| 11      | SH        |
| 12      | HS        |
| 13      | HS        |
| 14      | SH        |
| 15      | SH        |
| 16      | SH        |
| 17      | HS        |
| 18      | SH        |
| 19      | HS        |
| 20      | SH        |
| 21      | SH        |
| 22      | SH        |
| 23      | SH        |
| 24      | HS        |
| 25      | SH        |
| 26      | HS        |
| 27      | SH        |

Figure 5. Randomness for  $HS$  and  $SH$ .

Figure 5 shows the code used to create the block randomness for  $HS$  and  $SH$ . In the right part of the figure we can see the unique solution created by this blocked randomization code, where  $nna$  and  $nnb$  denote the number of  $H$ 's and  $S$ 's, respectively, to be contained with each block, supposing that when one value of Table 4 is already randomized to each group  $HS$  and  $SH$ , then:

$$P(HS) = \begin{cases} 0 & nna = na \\ \frac{nna-na}{nna+nnb-na-nb} & 0 < nna < nna. \\ 1 & nnb = nb \end{cases} \quad (23)$$

### Enthalpy vs. Entropy in Different Temperatures in a 2\*2 Crossover Trial Descriptive Statistics and Graphics for Sequence Difference Parametric Analysis

#### The TTEST Procedure

Variable: diff

| sequence   | Method        | N  | Mean    | Std Dev | Std Err | Minimum  | Maximum |
|------------|---------------|----|---------|---------|---------|----------|---------|
| HS         |               | 18 | 6453.2  | 5568.1  | 1312.4  | 377.2    | 18735.8 |
| SH         |               | 9  | -5916.2 | 4794.4  | 1598.1  | -14330.5 | 0       |
| Diff (1-2) | Pooled        |    | 12369.4 | 5332.8  | 2177.1  |          |         |
| Diff (1-2) | Satterthwaite |    | 12369.4 |         | 2068.0  |          |         |

| sequence   | Method        | Mean    | 95% CL Mean     | Std Dev | 95% CL Std Dev |
|------------|---------------|---------|-----------------|---------|----------------|
| HS         |               | 6453.2  | 3684.3 9222.2   | 5568.1  | 4178.2 8347.4  |
| SH         |               | -5916.2 | -9601.6 -2230.9 | 4794.4  | 3238.4 9185.1  |
| Diff (1-2) | Pooled        | 12369.4 | 7885.6 16853.2  | 5332.8  | 4182.3 7361.4  |
| Diff (1-2) | Satterthwaite | 12369.4 | 8032.8 16706.1  |         |                |

| Method        | Variances | DF     | t Value | Pr >  t |
|---------------|-----------|--------|---------|---------|
| Pooled        | Equal     | 25     | 5.68    | <.0001  |
| Satterthwaite | Unequal   | 18.475 | 5.98    | <.0001  |

| Equality of Variances |        |        |         |        |
|-----------------------|--------|--------|---------|--------|
| Method                | Num DF | Den DF | F Value | Pr > F |
| Folded F              | 17     | 8      | 1.35    | 0.6889 |

Figure 6. Sequence Difference of Enthalpy vs. Entropy.

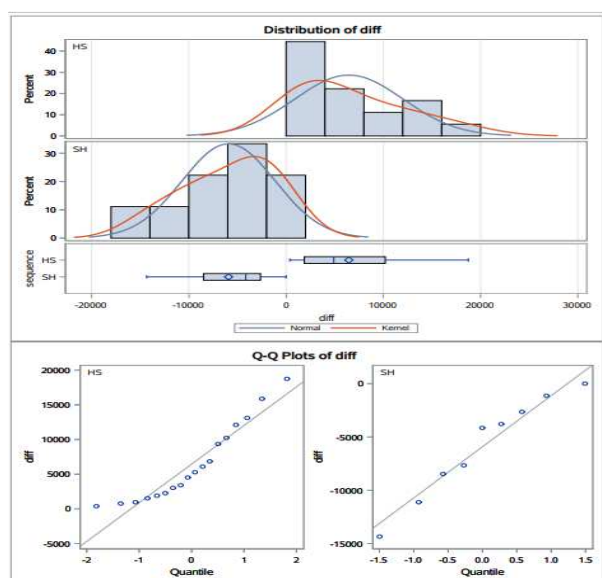


Figure 7. Descriptive Graphics for the Iceep *HS* and *SH*.

In Figure 6, we find the sequences for both groups. The pooled is the method to use when both variance are the same, if not, the Satterthwaite is given. In the second part, we see the results obtained with 95% confidence interval. In pooled, we assume the variance are equal, and in the Satterthwaite we assume the variance are unequal. We reject the null hypothesis, because it is not within our confidence interval, thus,  $H_0$  at  $p$ -value given at  $p = 0.0001$ .

In Figure 7, we can see in the first half the normal and kernel distributions for both *HS* and *SH*. In the second half all the points plotted are our actual numbers, and we assume both are equally distributed above and below the line (or all in the line), because the variances are assumed to be equal.

| Wilcoxon Scores (Rank Sums) for Variable diff<br>Classified by Variable sequence |    |               |                      |                     |            |
|----------------------------------------------------------------------------------|----|---------------|----------------------|---------------------|------------|
| sequence                                                                         | N  | Sum of Scores | Expected Under $H_0$ | Std Dev Under $H_0$ | Mean Score |
| HS                                                                               | 18 | 333.0         | 252.0                | 19.442222           | 18.50      |
| SH                                                                               | 9  | 45.0          | 126.0                | 19.442222           | 5.00       |

| Wilcoxon Two-Sample Test |         |        |         |                 |         |
|--------------------------|---------|--------|---------|-----------------|---------|
| Statistic                | Z       | Pr < Z | Pr >  Z | t Approximation |         |
|                          |         |        |         | Pr < Z          | Pr >  Z |
| 45.0000                  | -4.1405 | <.0001 | <.0001  | 0.0002          | 0.0003  |

Z includes a continuity correction of 0.5.

| Kruskal-Wallis Test |    |            |
|---------------------|----|------------|
| Chi-Square          | DF | Pr > ChiSq |
| 17.3571             | 1  | <.0001     |

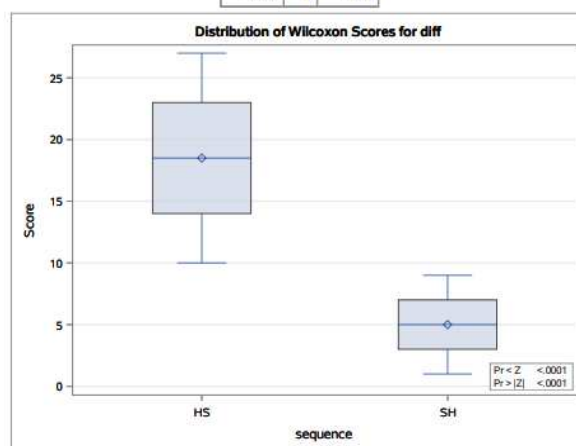


Figure 8. Non-parametric Results for Sequence *HS* and *SH*.

| Wilcoxon Scores (Rank Sums) for Variable Entropy<br>Classified by Variable sequence |    |               |                      |                     |            |
|-------------------------------------------------------------------------------------|----|---------------|----------------------|---------------------|------------|
| sequence                                                                            | N  | Sum of Scores | Expected Under $H_0$ | Std Dev Under $H_0$ | Mean Score |
| HS                                                                                  | 18 | 254.0         | 252.0                | 19.442222           | 14.111111  |
| SH                                                                                  | 9  | 124.0         | 126.0                | 19.442222           | 13.777778  |

| Wilcoxon Two-Sample Test |         |        |         |                 |         |
|--------------------------|---------|--------|---------|-----------------|---------|
| Statistic                | Z       | Pr < Z | Pr >  Z | t Approximation |         |
|                          |         |        |         | Pr < Z          | Pr >  Z |
| 124.0000                 | -0.0772 | 0.4693 | 0.9385  | 0.4695          | 0.9391  |

Z includes a continuity correction of 0.5.

| Kruskal-Wallis Test |    |            |
|---------------------|----|------------|
| Chi-Square          | DF | Pr > ChiSq |
| 0.0106              | 1  | 0.9181     |

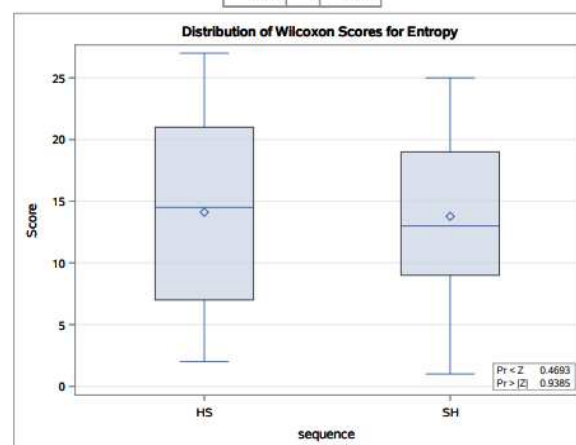


Figure 9. Parametric Results for Sequence *HS* and *SH*.

Assuming that the carryout effects are equal for both thermodynamic quantities, we compare both sequences with respect to their differences which to give us zero, this means there is not difference if both variances are equal. We start with a null hypothesis,  $H_0$  = no difference. We then reject this hypothesis if our  $p$ -value is in the rejection region. The result was a  $p$ -value in the rejection region which implies that we need to reject the null hypothesis. We can use this information to say that there are significant differences, then these two quantities are dependent to each other.

The next part is solved using the Chi-square table, because we can express the Maxwell distribution as the  $\chi^2$  distribution. For Table 4, with a total of 2 columns and 27 rows, the degree of freedom is 26, with  $\alpha = 0.05$  as the confidence region. Therefore, if  $\chi^2 \leq 38.89$ , we reject  $\chi^2$ . As before the null hypothesis,  $H_0$  = independent quantities and alternative hypothesis,  $H_1$  = dependent quantities.

For Table 4, the first entry at  $T = 0.01$  is going to be  $H = 0 = a_{1,1}$ , and second entry of our first row  $a_{1,2} = 0 = S$ . We continue with this sequence until row 27 has entries  $a_{27,1} = 37,551$  and  $a_{27,2} = 79.40$ . For  $\chi^2$ , we need to find  $C_{1,1}, C_{1,2}, \dots, C_{27,1}$ , and  $C_{27,2}$ , where

$$C_{r,c} = \frac{(\sum r_i)(\sum c_j)}{\sum r_i + \sum c_j}. \quad (24)$$

For example,  $C_{2,1} = (\text{sum of second row})(\text{sum of first column})$  divided by the total sum of all rows and columns. This gives  $C_{2,1} = \frac{(759.822)(339688.2)}{(340568.6)} = 753.4332$ ,  $C_{2,2} = \frac{(759.822)(880.397)}{(340568.6)} = 1.9642$ , and so on. Then the  $\chi^2$  statistic is calculated by using:

$$\chi^2 = \frac{(a_{1,1} - C_{1,1})^2}{C_{1,1}} + \dots + \frac{(a_{27,2} - C_{27,2})^2}{C_{27,2}}. \quad (25)$$

Our  $\chi^2$  statistic ends with a value 17.7128  $\in$  rejection region. Therefore, we reject the null hypothesis of  $H_0$  = independent quantities, to conclude the entropy and enthalpy are dependent of each other. We perform the same method to show dependence or independence for  $T$  vs.  $H$  and  $T$  vs.  $S$ . Note that we prefer to ignore our  $a_{1,1}, a_{1,2}, C_{1,1}$ , and  $C_{2,1}$  because enthalpy ( $H$ ) and entropy ( $S$ ) can only be measured with the change of their quantities. We start at  $T = 0.01$ , and we do not generate any values of  $\Delta H$  or  $\Delta S$ . Thus, the first row start with values of 0. Now, considering heat is a class of energy, and it is related to the speed of the particles in the system. We assume that there is a strong positive relation between temperature vs. enthalpy, temperature vs. entropy, and enthalpy vs. entropy.

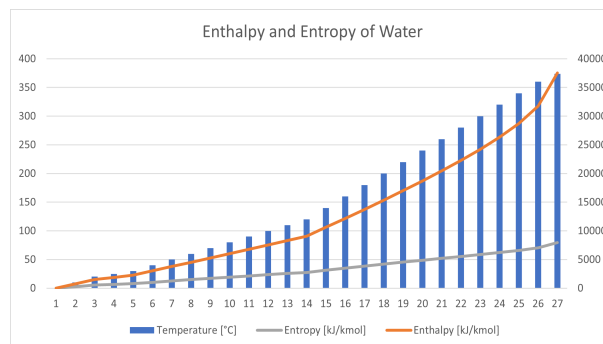


Figure 10. Graphs of Entropy and Enthalpy vs. Temperature.

Figure 10 shows the column graph resulting from Table 4, where Entropy and Enthalpy as the dependent variables of heat. As we can see, when the temperature increases both  $H$  and  $S$  increase.

We have observations of 27 subjects consisting of a dependent or response variable,  $y$  = Entropy and an explanatory variable,  $x$  = Enthalpy. If the Enthalpy of the system increases, it will make the Entropy increases as well. For the ratio estimation with two quantities  $y_i$  = Entropy, and  $x_i$  = Enthalpy we must measure each sample unit, where  $x_i$  is called an auxiliary variable in the sample size of  $n = 27$ ,

$$t_y = \sum_{i=1}^N y_i, \quad t_x = \sum_{i=1}^N x_i \quad (26)$$

with ratio given by

$$B = \frac{t_y}{t_x} \quad (27)$$

and covariance given by:

$$\text{cov}(x, y) = \text{cov}(y, x) = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{n - 1}. \quad (28)$$

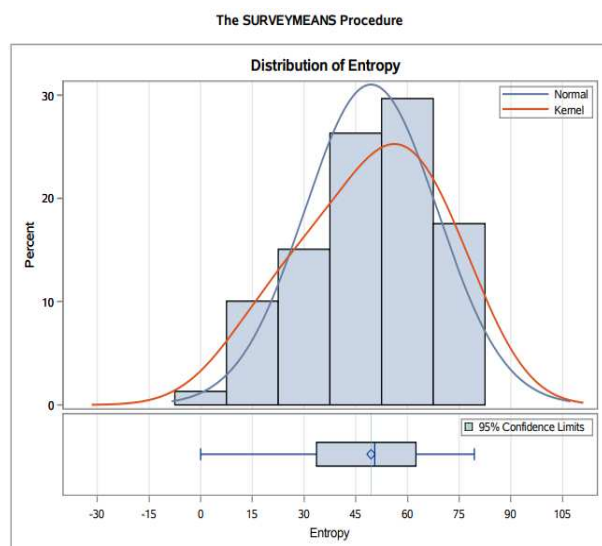
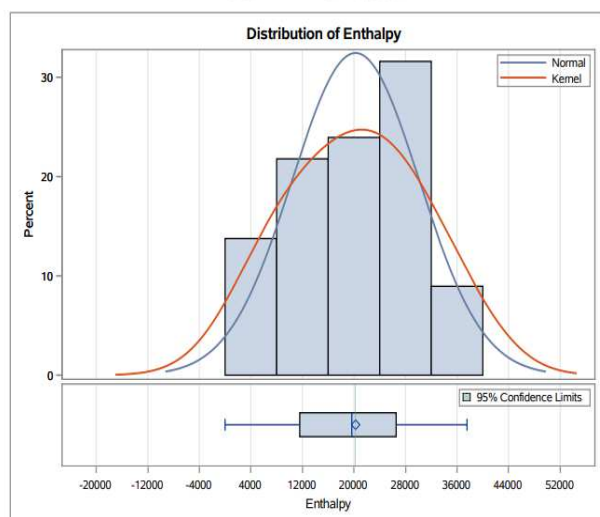
If  $\text{cov}(x, y) > 0$ , then there is a positive relationship between Entropy and Enthalpy, but if  $\text{cov}(x, y) < 0$ , then the relationship is negative, we define the sample correlation coefficient  $R$  as

$$R = \frac{\sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})}{(N - 1)(S_x S_y)}, \quad (29)$$

where  $S_x$  is the standard deviation for  $x_i$  and  $S_y$  is the standard deviation for  $y_i$ .

From Table 4, the total for the sum of  $x_i$  is given by  $t_x = 0 + 757.1 + \dots + 31,739 + 37,551 = 339,688.2$ , and mean  $\bar{x} = 12,581.044$ . The total for the sum of  $y_i$  is given by  $t_y = 0 + 2.722 + 5.341 + \dots + 70.56 + 79.4 = 880.077$  and mean  $\bar{y} = 32.595$ .  $S_x = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n - 1}} = 10,493.808$ .  $S_y = \sqrt{\frac{\sum (y_i - \bar{y})^2}{n - 1}} = 22.886$ . The ratio  $B = \frac{t_y}{t_x} = 0.003$ . The covariance,  $\text{cov}(x, y) = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{n - 1}$  equal 238,115.1

means our sample have a positive relation. With all these values we are able to find the correlation population coefficient as  $R = \frac{6,190,993}{(27-1)(10,493.80775)(22.886)} = 0.992$ . The relation is stronger as  $R$  is close to 1.

Distribution of Entropy ( $S$ )Distribution of Enthalpy ( $H$ )Figure 11. Comparison of Entropy ( $S$ ) and Enthalpy ( $H$ ) Distributions.

In Figure 11, the left side distribution shows that this distribution of Entropy is slightly skewed to the right. That is to say that there are fewer lower valued Entropy in the distribution. Both distributions are the results from the data provided in Table 4. The blue line are for the normal distribution and the red line is for the kernel distribution that control the smoothness of the resulting density curve for both entropy and enthalpy.

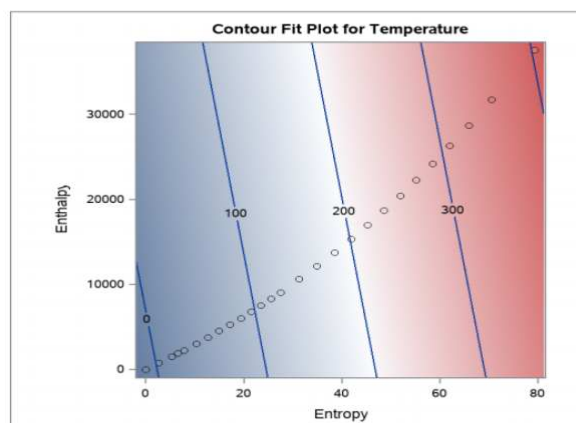


Figure 12. Contour Fitting for Temperature for Known Band Entropy and Enthalpy.

A surface and contour fit plot of temperature for known Bend Entropy and Enthalpy divided into three surfaces at 100°C, 200°C, and 300°C contours are provided in Figure 13.

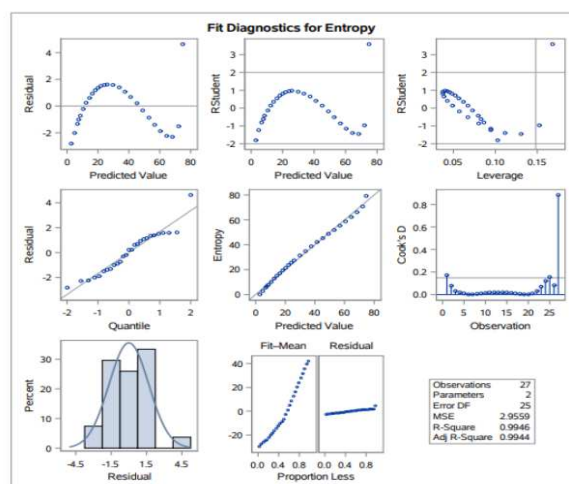


Figure 13.A. The REG procedure with dependent variable Entropy.

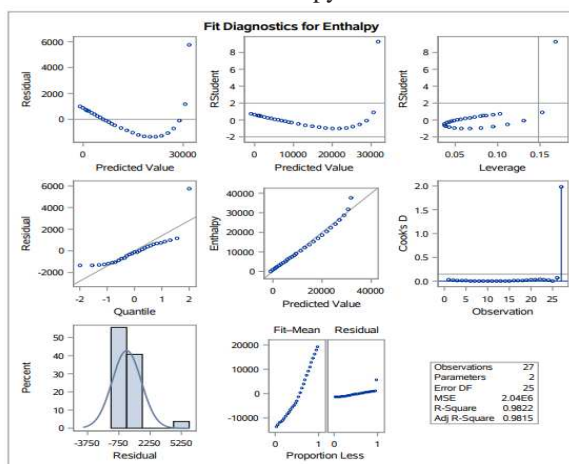


Figure 13.B. The REG procedure with dependent variable Enthalpy.

On the left side, REG procedure with dependent variable Entropy, they are the nine model selected methods are available in PROC REG. PROC REG fits the complete model that is specified. The other eight methods involve various ways of including or excluding variables from the model from col-linearity diagnostics. This is done for both Entropy and Enthalpy. Each chart utilizes 27 observation points restricted to two separate parameters. The data generated a mean squared error (MSE) of 2.956, R-square of 0.995, and adjusted R-square of 0.994, and nine model selected methods are available in PROC REG. For the dependent variable Enthalpy the PROC REG fits the complete model that is specified. The data generated a mean squared error (MSE) of  $2.04 \times 10^6$ , R-square of 0.982, and adjusted R-square of 0.982 as we can see in Figures 14.A and 14.B.

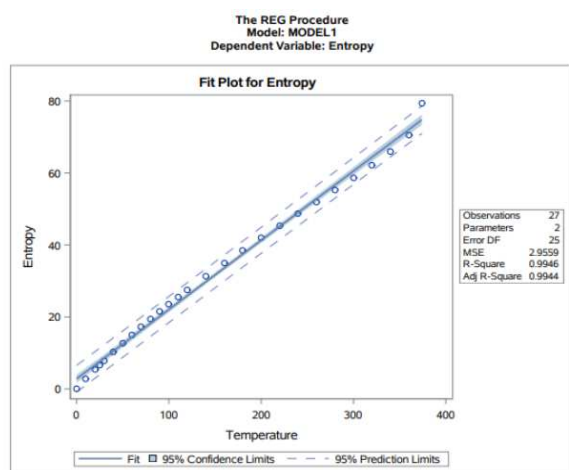


Figure 14.A. Linear regression for Entropy and temperature in water.

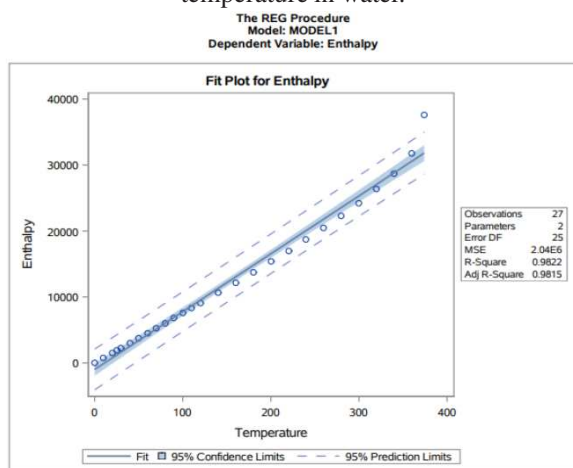


Figure 14.B. Linear Regression for Enthalpy and Temperature in Water.

In the left image of Figures 14.A and 14.B, we can appreciate a strong linear regression between temperature and Entropy that follows the linear equation  $y = 87.673x - 988.683$ , where  $y$  = Entropy is the dependent variable of  $x$

= temperature, the independent variable. In the right image, we have a strong linear regression between temperature and Enthalpy that follows the equation  $y = 0.192x + 2.816$ , where  $y$  = enthalpy is the dependent variable of  $x$  = temperature, the independent variable.

The Avogadro's number tells us that there are  $6.022 \times 10^{23}$  molecules of water per mole. At room temperature ( $20^\circ\text{C}$  or  $68^\circ\text{F}$ ) the mean speed of the water molecules is approximately 590 m/s or 1,300 mph. Roughly 50%, ( $3.011 \times 10^{23}$ ) of molecules of the water per mole of water, travels with a speed between 400 m/s and 740 m/s. One fourth,  $1.506 \times 10^{23}$  per mole of water, have a velocity less than 400 m/s, and the remaining 25% have a speed greater than 740 m/s, as follows from the Maxwell-Boltzmann distribution. This describes the distribution of the speeds of the water molecules when the water is in thermodynamic equilibrium.

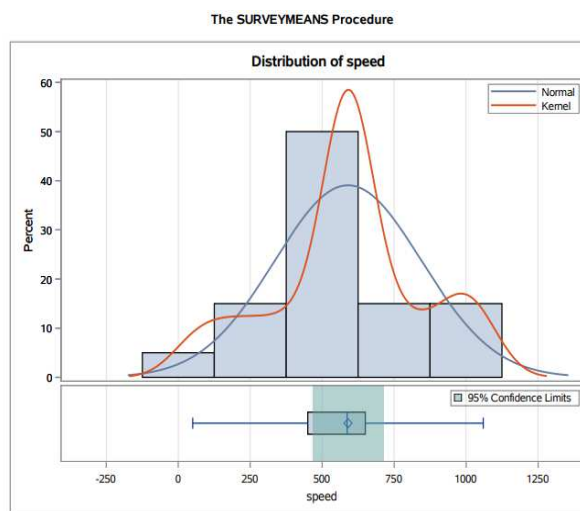


Figure 15. Speed Distribution of Particles in Water at  $20^\circ\text{C}$ .

At this room temperature ( $20^\circ\text{C}$ ), the Enthalpy of water is around 1,511.8 kJ/kmol, and the Entropy is around 5.341 kJ/kmol. It shows that speed distribution is slightly left-skewed.

Table 5. Mean Results for the Data in Table 4.

| The MEANS Procedure       |             |             |            |         |
|---------------------------|-------------|-------------|------------|---------|
| Analysis Variable : Speed |             |             |            |         |
| N                         | Mean        | Std Dev     | Minimum    | Maximum |
| 20                        | 590.0000000 | 261.8557256 | 50.0000000 | 1060.00 |

Table 5 is the mean result for 20 random particles in water at  $20^\circ\text{C}$ . The mean tells us that most of the particle have a speed of  $590 \frac{\text{m}}{\text{s}}$  at room temperature, where the distribution speed of particles reach the highest point for probability as shows in Figure 15.

Table 6. Frequency Procedure Implemented for Speed Distribution.

The FREQ Procedure

| Speed | Frequency | Percent | Cumulative Frequency | Cumulative Percent |
|-------|-----------|---------|----------------------|--------------------|
| 50    | 1         | 5.00    | 1                    | 5.00               |
| 150   | 1         | 5.00    | 2                    | 10.00              |
| 250   | 1         | 5.00    | 3                    | 15.00              |
| 350   | 1         | 5.00    | 4                    | 20.00              |
| 450   | 1         | 5.00    | 5                    | 25.00              |
| 550   | 1         | 5.00    | 6                    | 30.00              |
| 580   | 2         | 10.00   | 8                    | 40.00              |
| 590   | 3         | 15.00   | 11                   | 55.00              |
| 600   | 3         | 15.00   | 14                   | 70.00              |
| 650   | 1         | 5.00    | 15                   | 75.00              |
| 750   | 1         | 5.00    | 16                   | 80.00              |
| 850   | 1         | 5.00    | 17                   | 85.00              |
| 960   | 1         | 5.00    | 18                   | 90.00              |
| 1000  | 1         | 5.00    | 19                   | 95.00              |
| 1060  | 1         | 5.00    | 20                   | 100.00             |

Table 6 is the frequency table of 20 particles in water at 20°C (for 20 simple random samples choosing from the whole particles).

Table 7. UNI-VARIATE Procedure for the Speed Distribution at 20 C.

The UNIVARIATE Procedure  
Variable: Speed  
Molecules = 0.3011

| Moments         |            |                  |            |
|-----------------|------------|------------------|------------|
| N               | 20         | Sum Weights      | 20         |
| Mean            | 590        | Sum Observations | 11800      |
| Std Deviation   | 261.855726 | Variance         | 68568.4211 |
| Skewness        | -0.1735915 | Kurtosis         | 0.15775487 |
| Uncorrected SS  | 8264800    | Corrected SS     | 1302800    |
| Coeff Variation | 44.3823264 | Std Error Mean   | 58.5527203 |

| Basic Statistical Measures |          |                     |           |
|----------------------------|----------|---------------------|-----------|
| Location                   |          | Variability         |           |
| Mean                       | 590.0000 | Std Deviation       | 261.85573 |
| Median                     | 590.0000 | Variance            | 68568     |
| Mode                       | 590.0000 | Range               | 1010      |
|                            |          | Interquartile Range | 200.00000 |

Note: The mode displayed is the smallest of 2 modes with a count of 3.

| Tests for Location: $\mu_0=0$ |           |          |          |        |
|-------------------------------|-----------|----------|----------|--------|
| Test                          | Statistic | p Value  |          |        |
| Student's t                   | t         | 10.07639 | Pr >  t  | <.0001 |
| Sign                          | M         | 10       | Pr >=  M | <.0001 |
| Signed Rank                   | S         | 105      | Pr >=  S | <.0001 |

There is a change in the velocity of the molecules of water at 0°C, which is the temperature when the water start freezing. The mean at this temperature is 565 m/s (1250 mph), whose means the molecules start moving slower. On the other hand, 100°C which is the boiling point of water, the speed of the molecules increases, reaching a mean of 660 m/s (1500 mph). As we can see below, the data corresponding at 0°C is represented to the left, and the data corresponding at 100°C is represented to the right.

Table 8. Frequency of Particles of Water at 0°C and 100°C.

The FREQ Procedure

| Speed | Frequency | Percent | Cumulative Frequency | Cumulative Percent |
|-------|-----------|---------|----------------------|--------------------|
| 20    | 1         | 5.00    | 1                    | 5.00               |
| 80    | 1         | 5.00    | 2                    | 10.00              |
| 190   | 1         | 5.00    | 3                    | 15.00              |
| 250   | 2         | 10.00   | 5                    | 25.00              |
| 360   | 1         | 5.00    | 6                    | 30.00              |
| 480   | 1         | 5.00    | 7                    | 35.00              |
| 530   | 1         | 5.00    | 8                    | 40.00              |
| 540   | 1         | 5.00    | 9                    | 45.00              |
| 550   | 1         | 5.00    | 10                   | 50.00              |
| 570   | 1         | 5.00    | 11                   | 55.00              |
| 580   | 1         | 5.00    | 12                   | 60.00              |
| 630   | 1         | 5.00    | 13                   | 65.00              |
| 730   | 1         | 5.00    | 14                   | 70.00              |
| 830   | 1         | 5.00    | 15                   | 75.00              |
| 840   | 1         | 5.00    | 16                   | 80.00              |
| 880   | 1         | 5.00    | 17                   | 85.00              |
| 940   | 1         | 5.00    | 18                   | 90.00              |
| 950   | 1         | 5.00    | 19                   | 95.00              |
| 1100  | 1         | 5.00    | 20                   | 100.00             |

The FREQ Procedure

| Speed | Frequency | Percent | Cumulative Frequency | Cumulative Percent |
|-------|-----------|---------|----------------------|--------------------|
| 10    | 1         | 5.00    | 1                    | 5.00               |
| 70    | 1         | 5.00    | 2                    | 10.00              |
| 170   | 1         | 5.00    | 3                    | 15.00              |
| 310   | 1         | 5.00    | 4                    | 20.00              |
| 390   | 1         | 5.00    | 5                    | 25.00              |
| 450   | 1         | 5.00    | 6                    | 30.00              |
| 560   | 1         | 5.00    | 7                    | 35.00              |
| 590   | 1         | 5.00    | 8                    | 40.00              |
| 630   | 1         | 5.00    | 9                    | 45.00              |
| 650   | 1         | 5.00    | 10                   | 50.00              |
| 670   | 1         | 5.00    | 11                   | 55.00              |
| 690   | 1         | 5.00    | 12                   | 60.00              |
| 740   | 1         | 5.00    | 13                   | 65.00              |
| 800   | 1         | 5.00    | 14                   | 70.00              |
| 910   | 1         | 5.00    | 15                   | 75.00              |
| 960   | 1         | 5.00    | 16                   | 80.00              |
| 1000  | 1         | 5.00    | 17                   | 85.00              |
| 1100  | 1         | 5.00    | 18                   | 90.00              |
| 1200  | 1         | 5.00    | 19                   | 95.00              |
| 1300  | 1         | 5.00    | 20                   | 100.00             |

The frequencies in Table 8 are the results of selecting 20 simple random samples of particles of water at a given temperature.

Table 9. Mean Results from Table 8.

The MEANS Procedure

| Analysis Variable : Speed |             |             |            |         |
|---------------------------|-------------|-------------|------------|---------|
| N                         | Mean        | Std Dev     | Minimum    | Maximum |
| 20                        | 565.0000000 | 305.6055249 | 20.0000000 | 1100.00 |

The MEANS Procedure

| Analysis Variable : Speed |             |             |            |         |
|---------------------------|-------------|-------------|------------|---------|
| N                         | Mean        | Std Dev     | Minimum    | Maximum |
| 20                        | 660.0000000 | 359.5318594 | 10.0000000 | 1300.00 |

Table 10. UNI-VARIATE Procedure for the Speed Distribution at 0°C and 100°C.

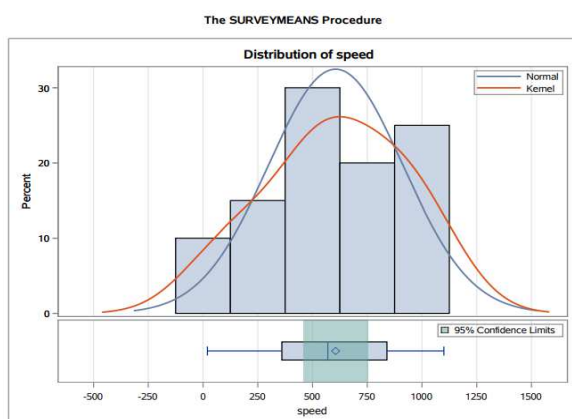
| The UNIVARIATE Procedure |            |                  |            | The UNIVARIATE Procedure |            |                  |            |
|--------------------------|------------|------------------|------------|--------------------------|------------|------------------|------------|
| Variable: Speed          |            |                  |            | Variable: Speed          |            |                  |            |
| Molecules = 0.3011       |            |                  |            | Molecules = 0.3011       |            |                  |            |
| Moments                  |            |                  |            | Moments                  |            |                  |            |
| N                        | 20         | Sum Weights      | 20         | N                        | 20         | Sum Weights      | 20         |
| Mean                     | 565        | Sum Observations | 11300      | Mean                     | 660        | Sum Observations | 13200      |
| Std Deviation            | 305.60525  | Variance         | 93394.7368 | Std Deviation            | 359.53186  | Variance         | 129263.158 |
| Skewness                 | -0.1273103 | Kurtosis         | -0.8081161 | Skewness                 | -0.1017202 | Kurtosis         | -0.5310099 |
| Uncorrected SS           | 8159000    | Corrected SS     | 1774500    | Uncorrected SS           | 11168000   | Corrected SS     | 2456000    |
| Coeff Variation          | 54.0894734 | Std Error Mean   | 68.3354728 | Coeff Variation          | 54.4745241 | Std Error Mean   | 80.3937678 |

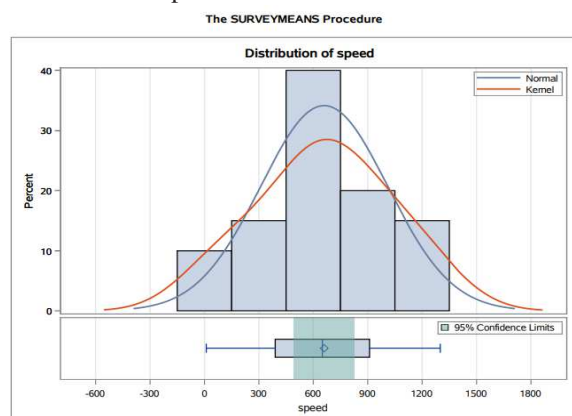
| Basic Statistical Measures |          |                     |           | Basic Statistical Measures |          |                     |           |
|----------------------------|----------|---------------------|-----------|----------------------------|----------|---------------------|-----------|
| Location                   |          | Variability         |           | Location                   |          | Variability         |           |
| Mean                       | 565.0000 | Std Deviation       | 305.6052  | Mean                       | 660.0000 | Std Deviation       | 359.53186 |
| Median                     | 560.0000 | Variance            | 93395     | Median                     | 660.0000 | Variance            | 129263    |
| Mode                       | 250.0000 | Range               | 1080      | Mode                       | .        | Range               | 1290      |
|                            |          | Interquartile Range | 530.00000 |                            |          | Interquartile Range | 515.00000 |

| Tests for Location: Mu0=0 |           |          |          | Tests for Location: Mu0=0 |           |          |          |
|---------------------------|-----------|----------|----------|---------------------------|-----------|----------|----------|
| Test                      | Statistic | Pr >  t  | p Value  | Test                      | Statistic | Pr >  t  | p Value  |
| Student's t               | t         | 8.268034 | Pr >  t  | Student's t               | t         | 8.209592 | Pr >  t  |
| Sign                      | M         | 10       | Pr >=  M | Sign                      | M         | 10       | Pr >=  M |
| Signed Rank               | S         | 105      | Pr >=  S | Signed Rank               | S         | 105      | Pr >=  S |



Speed Distribution at 0°C.



Speed Distribution at 100°C.

Figure 16. Comparison of Distribution 0°C vs. 100°C.

When heat is applied to the ice, it increases its temperature but never exceeds 0°C, from there it is

transformed into water, in the same way the water does not exceed 100°C since from there it turns into steam. At 0°C both the enthalpy and entropy of water are close to zero. Meanwhile, at 100°C the enthalpy is around 7,551.8 kJ/kmol, and entropy is around 23.55 kJ/kmol. This is the reason why the gaseous state gives us a better use of the energy of the system.

Table 11. Correlation Procedure for Entropy and Enthalpy.

| The CORR Procedure |  |          |  |  |  |  |
|--------------------|--|----------|--|--|--|--|
| 1 With Variables:  |  | Entropy  |  |  |  |  |
| 1 Variables:       |  | Enthalpy |  |  |  |  |

| Simple Statistics |    |          |          |           |         |          |
|-------------------|----|----------|----------|-----------|---------|----------|
| Variable          | N  | Mean     | Std Dev  | Sum       | Minimum | Maximum  |
| Entropy           | 27 | 32.59544 | 22.88554 | 880.07700 | 0       | 79.40000 |
| Enthalpy          | 27 | 12581    | 10494    | 339688    | 0       | 37551    |

| Pearson Correlation Coefficients, N = 27 |  | Prob >  r  under H0: Rho=0 |        |
|------------------------------------------|--|----------------------------|--------|
|                                          |  | Enthalpy                   |        |
| Entropy                                  |  | 0.99150                    | <.0001 |

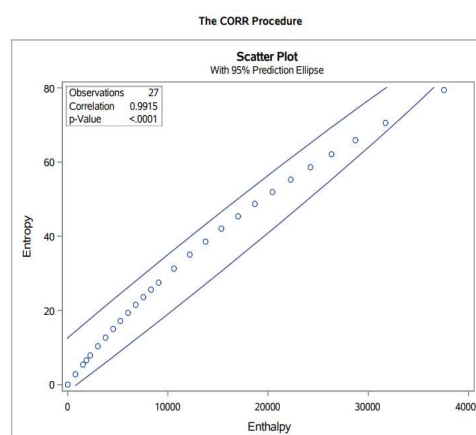


Figure 17. Correlation between Enthalpy and Entropy.

The correlation between entropy and enthalpy in water along different temperatures was calculated to be approximately 0.9915. This shows that there is a strong positive correlation between the two variables and is given by the following linear function:

$$y = 0.002x + 5.391.$$

We know that the more energy (heat) there in a system, the greater its entropy, but as the entropy increases, the enthalpy also increases proportionally taking a good amount of free energy from the system [22].

## 4.2 Quantum Physics

The temperature of atomic cloud is  $300\mu K$ , and the lifetime is longer than 50s. The temperature of atoms from up to down is respectively  $1.44\mu K$ ,  $320nK$ ,  $230nK$ , and  $120nK$ . The relation between the effective axial size and the temperature of the atomic cloud is in tight confinement and the velocity distribution along the  $v_y$  direction in the cross section of  $v_z = 15.68cm/s$  [23].

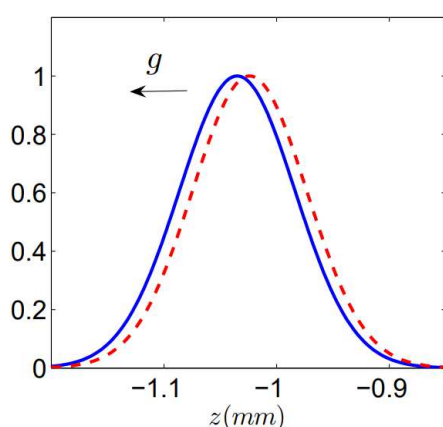


Figure 18.A. Simulation of the effect with  $z$   
 $V_z (cm s^{-1})$

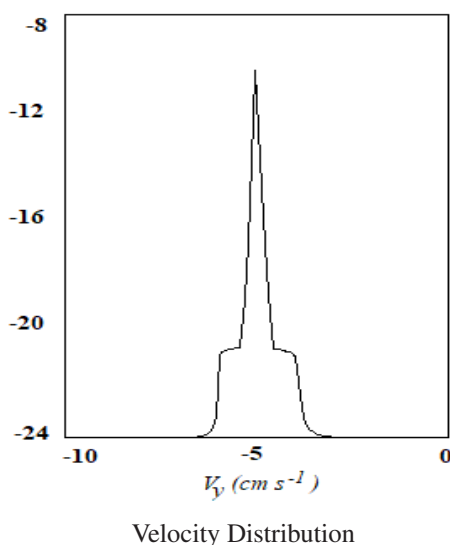


Figure 18.B. Velocity Distribution with its Simulation of kernel Effect with  $Z$ .

Figures 18.A and 18.B, represents simulation of the advance effect along the  $z$  direction. The dashed curve plots the cold atomic clouds free fall in the gravity field, and the solid curve shows the atomic cloud as it traverses through the Gaussian light beam in the gravity field. Figure 18.B. is similar to Figure 3, the distribution is shifted to higher speed and is broadened at the higher temperatures [24].

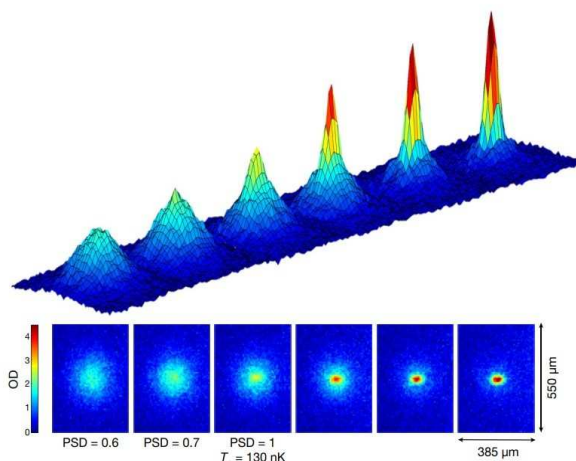


Figure 19. Bose-Einstein Condensate.

Figure 19 from University of Colorado, Boulder much is needed edition to Mike Matthews of the JILA research team. It concluded that Bose-Einstein condensate is the entropy decreases until it reaches its “minimum.” In other words, a Bose-Einstein condensates is the minimum state of entropy in a system of bosons.

## 5 Conclusions

We conclude the entropy depends on the standard deviation of the distribution. A high value of standard deviation means a high value of Entropy. For the case of finding a really low value of the entropy the standard deviation have to be insignificant. At normal temperatures, for example at  $20^\circ C$ , the wave associated with the particles is very small, and if we have a boson gas, the size of the waves of each of these particles will be less than the distance between them. Each particle, with its wave, occupies a region of space, they are separated and the particles do not interact with each other and each particle has an individual behavior, but as we reduce the temperature of the system, the wavelength associated with each particle increases as depicted as Figure 19. In the vicinity of absolute zero they overlap, beginning to interact with each other, interfering and forming a joint wave working as a single atom or super atom. Using the Maxwell and Boltzmann classical statistics, where we split our system into numerous cells, we predict how to arrange all the particles in those cells. By putting the system in temperatures close to absolute zero, this ends with a single distribution without the discrepancy of standard deviation or entropy.

## 6 Future Research

The applications of the Bose-Einstein condensates are at the moment endless. At present the study is extremely important, because as when the electronic properties of

metals were discovered or of the gaseous state used in factories, cars, refrigerators, steam engines and much more. The Bose-Einstein condensates could open the doors to the future in gravitational wave studies in ways other than LIGO detectors as in Figure 19. It will open up techniques such as superfluidity or superconductivity, and possibly more applications that at the moment we cannot even imagine. The 20th century has known scientific revolutions such as quantum physics and the theory of relativity, and yet after a century and a half the laws of thermodynamics are still one of the pillars of physics.

## 7 Discussion

All matter, whether solid, liquid or gaseous, is composed of atoms and molecules. These particles are not immobile, but they move more easily depending on their state. Heat is always transmitted exponentially from the body with the highest temperature to the lowest temperature, regardless of the total heat of each body. We know that taking advantage of heat is vital for daily use and could have better uses in the future, and we also know that entropy is the energy that we cannot use to create work. We wonder if there is a way to reduce the entropy of a system. The entropy of one system may decrease as the entropy of another system increases. This is why it is easier to study superconductivity in materials when they are placed at temperatures close to absolute zero.

## Acknowledgement

The first author has undertaken preliminary work of this research project during the coursework of STAT 5390-190 Case Seminar in Applied Statistics in Fall 2020 and continued the project for the completion during the coursework of MATH 4395-290 Senior Mathematics Project in Spring 2021 at the direction of Dr. Rohitha Goonatilake at Texas A&M International University (TAMIU), Laredo, Texas. The authors would like to thank Dr. Juan H. Hinojosa, who were immensely involved in the preliminary draft of the paper.

## References

- [1] T. L. Hill. Ensembles and Postulates, in *An Introduction to Statistical Thermo-dynamics*, Dover Publications, Ed. New York: 3-4, (2007).
- [2] J. Lucas. What Is the Second Law of Thermodynamics? LiveScience, (2015). <https://www.livescience.com/50941-second-law-thermodynamics.html>.
- [3] S. Chib and I. Jeliaskov. Marginal Likelihood from the Metropolis – Hastings Output. *Journal of the American Statistical Association*, 96, 270-281, (2001).
- [4] S. Vitoratou and I. Ntzoufras. Thermodynamic Bayesian model comparison. *Statistics and Computing*, 27, 1165-1180, (2017).
- [5] D. Lowe. Enthalpy and Entropy Again. *Science*, (2010). <https://www.science.org/content/blog-post/enthalpy-and-entropy-again>.
- [6] J. B. Chaires. Calorimetry and Thermodynamics in Drug Design. *Annual Reviews*, 37, 135-151, (2008).
- [7] D. J. Amit and Y. Verbin. *Statistical physics: An Introduction Course*, World Scientific Publishing Company, (1999).
- [8] T. Ruggeri and M. Sugiyama. *Rational Extended Thermodynamics beyond the Monatomic Gas*. Springer, (2015).
- [9] *Equilibrium and Advanced Thermodynamics Balances in Chemical Reactions*, Annenberg Learner, (2019). <https://www.learner.org/series/chemistry-challenges-and-solutions/equilibrium-and-advanced-thermodynamics-balance-in-chemical-reactions/>.
- [10] *Equilibrium and Advanced Thermodynamics Balances in Chemical Reactions*, Annenberg Learner, (2019).
- [11] T. Ruggeri and M. Sugiyama. *Rational Extended Thermodynamics beyond the Monatomic Gas*. Springer, (2015).
- [12] P. Jizba and J. Korbelt. Maximum Entropy Principle in statistical inference: case for non-Shannonian entropies. *Cornell University*, 1-12, (2018).
- [13] H. Kaur. Maxwell-Boltzmann Statistics. SlidePlayer, (2016). <https://slideplayer.com/slide/6262040/>.
- [14] M. Grzegorzczak, A. Aderhold, and D. Husmeier. Targeting Bayes factors with direct-path non-equilibrium thermodynamic integration, *Computational Statistics*, 32, 717-761, (2017).
- [15] M. S. Tabass and G. R. M. Borzadaran. The generalized maximum Tsallis entropy estimators and applications to the Portland cement dataset. *Communications in Statistics – Simulation and Computation*, 46, 3284-3293, (2015).
- [16] M. G. Bulmer. *Principle of Statistics* (Dover Books of Mathematics). Dover Publications, (1979).
- [17] Water - Enthalpy (H) and Entropy (S). Engineering ToolBox, (2009). [https://www.engineeringtoolbox.com/water-properties-d\\_1508.html](https://www.engineeringtoolbox.com/water-properties-d_1508.html).
- [18] P. E. Matthews. *Bose-Einstein Condensates: Theory, Characteristics, and current research* (Physics Research and Technology). Nova Science, UK, (2010).
- [19] H. Hernandez. On the generalized validity of the Maxwell-Boltzmann distribution and the zeroth Law of Thermodynamics. *ForsChem Research Reports*, 1-11, (2016).
- [20] S. N. Bose. Plancks Gesetz und Lichtquantenhypothese. *Zeitschrift für Physik*, 26, 178-181, (1924).
- [21] Water - Enthalpy (H) and Entropy (S). Engineering ToolBox, (2009).
- [22] W. Moebs, S. J. Ling, and J. Sanny. *University Physics: Volume 2 and 3*. Openstax, Houston TX, (2016).
- [23] M. R. Matthews, D. S. Hall, D. S. Jin, J. R. Ensher, C. E. Wieman, E. A. Cornell, F. Dalfovo, C. Minniti, and S. Stringari. Dynamical Response of a Bose-Einstein Condensate to a Discontinuous Change in Internal State. *Physical Review Letters*, 81, 243, (1998).
- [24] *Molecular Speed Distribution*. Grade 7 Vertical Science, (2011). <https://www.verticallearning.org/curriculum/science/gr7/student/unit01/page05.html>.