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Article

Investigation of the total entropy for carbon dioxide gas with a constant Temperature condition

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Abstract. The amount of thermal energy per unit of temperature in a system that cannot be used to carry out beneficial work is known as entropy. Entropy is a measure of a system's molecular disorder or unpredictability since work is produced by organized molecular motion. It aids in figuring out an object's thermodynamic condition. A little thought will reveal that a spontaneous process shifts from a less probable condition to a more probable state when it occurs. It expresses the condition of a body in the same way as temperature, pressure, volume, internal energy, and magnetic behavior. So, in this work, the entropy details of the CO2 gas at various pressure and temperature conditions are discussed. It was observed that the entropy of the system is highly dependent on the pressure of the gas in a closed system. Also, the entropy is directly proportional to the pressure of the gas.

Keywords: CO2 gas, Thermodynamic Equilibrium, Entropy

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1. Introduction

Physics' discipline of thermodynamics deals with a system's energy and work.[1] The study of propulsion systems and comprehending high speed flows are two areas of aerodynamics in which we are most interested in thermodynamics. According to the first law of thermodynamics, a system's overall energy is conserved. The system's work, heat transfer, potential and kinetic energy, and kinetic energy are all included in the total energy.[2] While numerous physical processes that satisfies the first condition are possible, according to the second law of thermodynamics, the only processes that happen in nature are those for which the entropy of the system either remains constant or increases.[3,4]

The fact that the idea of entropy has consistently attracted errors and misinterpretations that have left the idea bruised, bleeding, and unrecognizably altered is maybe appropriate. Although it is not immediately apparent, the incorrect portrayal of entropy has a significant impact on current educational events, particularly in national and international discussions about the teaching of evolution.[5,6] The theory of evolution by natural selection was initially put forth and has mostly been improved through the preceding two centuries, similar to the concept of entropy.

Presenting teachable opportunities to clarify the idea of entropy and associated fallacies about evolution that are frequently used in conjunction with misinterpretations of entropy is the current abuse of thermodynamics and entropy in arguments against evolution.[7,8] In order to accomplish this, we provide a historical overview of the idea of entropy in the context of thermodynamics, offer a simple definition of entropy with examples that can be utilized in a classroom setting, and talk about how entropy truly relates to and supports the theory of evolution.

The fundamental idea in thermodynamics and statistical mechanics is Entropy. Around a century ago, Clausius, Kelvin, Maxwell, Boltzmann, and many others recognized its suzerain function in determining the behaviour of macroscopic systems.[9,10] The fact that most of the key entropy characteristics are mostly unknown to physicists and that many entropy-related issues are still unresolved or have just recently been resolved is therefore quite astounding. Entropy is a measurable physical characteristic and a scientific notion that is frequently connected to a condition of disorder, unpredictability, or uncertainty. From classical thermodynamics, where it was originally recognized, through the microscopic description of nature in statistical physics, to the fundamentals of information theory, the phrase and concept are utilized in a variety of disciplines. It has numerous applications in physics and chemistry, biological systems and how they relate to life, cosmology, economics, sociology, weather science, and information systems, especially the exchange of information.[11]

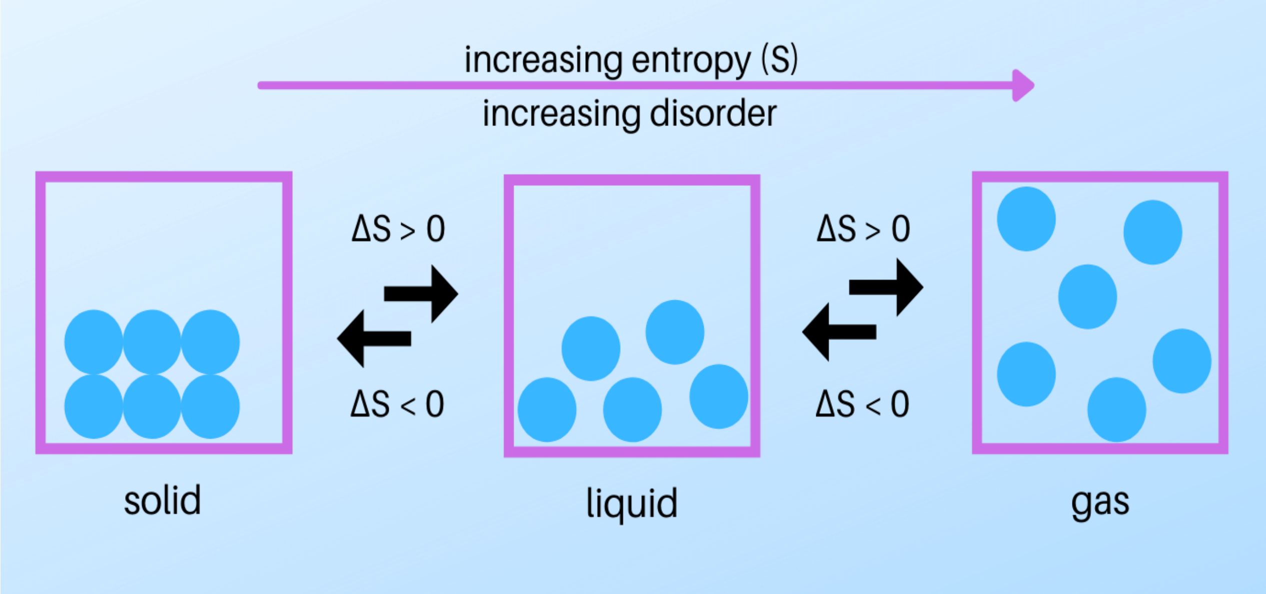

Figure 1: Simple demonstration of entropy

Entropy links the macro- and microcosmic facets of nature and controls the behaviour of macroscopic systems, or real matter, when they are in equilibrium or nearly so. [12–14]Despite the efforts of countless scientists over the course of a century, it is still not fully understood why this is the case. There are numerous ideas and suggestions about how to solve this issue, but none of them seem to be entirely suitable. Entropy has the effect of making some processes impossible or irreversible, in addition to the need that they do not go against the conservation of energy, which is described in the first law of thermodynamics. The second law of thermodynamics, which asserts that isolated systems left to spontaneous development cannot have their entropy decrease over time because they always reach a state of thermodynamic equilibrium where it is highest, is based on the concept of entropy.

Scottish scientist and engineer Macquorn Rankine first used the terms' thermodynamic function and heat potential to describe the thermodynamic notion in 1850. The definition of thermodynamics given in 1865 by German physicist Rudolf Clausius, one of the principal pioneers of the discipline, is the ratio of an infinitesimal amount of heat to the immediate temperature. He first referred to it as transformation-content, or Verwandlungsinhalt, in German, and then adopted the Greek word for transformation to create the term entropy. Clausius defined the term "disgregation" in 1862 by referring to microscopic constitution and structure. Ludwig Boltzmann, an Austrian physicist, defined entropy as the count of microscopic configurations or states of individual atoms and molecules of a system that satisfy the macroscopic condition of the system. By doing so, he created a new branch of thermodynamics known as statistical mechanics and introduced the ideas of statistical disorder and probability distributions. He also discovered the connection between microscopic interactions, which fluctuate around an average configuration, and macroscopically observable behaviour in the form of a straightforward logarithmic law with a proportionality constant, the Boltzmann constant, which has since become one of the defining universal constants for the modern Interna (SI).[15,16]

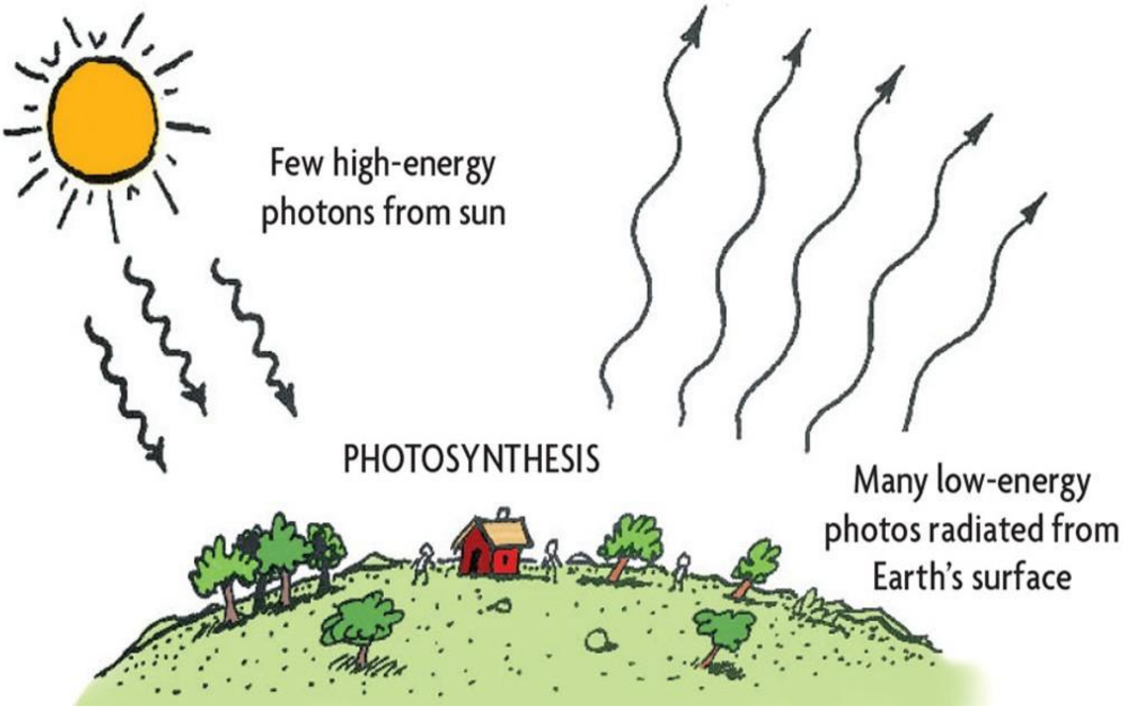

Figure 2: Simple nature application of entropy

Rudolf Clausius created the thermodynamic definition of entropy in the early 1850s, which effectively explains how to calculate the entropy of an isolated system that is in thermodynamic equilibrium with its constituent elements. Entropy is a broad thermodynamic variable that Clausius coined and demonstrated to be useful in describing the Carnot cycle. It was discovered that the relationship between heat transport and a system's temperature along the isotherm phases of the Carnot cycle (known as its absolute temperature). The incremental heat transfer divided by temperature ratio, which was discovered to change throughout the thermodynamic cycle but finally returns to the same value at the end of every cycle, was used to illustrate this relationship. The system's thermodynamic state, in particular, was found to be a function of the state as a result. Although Clausius founded his description on a reversible process, entropy can also vary as a result of irreversible processes. According to the second rule of thermodynamics, for irreversible processes, the entropy of an isolated system constantly rises. Energy may not flow to or from an isolated system, but it is feasible for energy to do so from a closed system, which is the difference between them. However, irreversible thermodynamic processes can happen in both closed and isolated systems, as well as in open systems.[17,18]

A reaction that is energy-wise viable but not necessarily likely to occur is one that is possible. Although it would be possible energetically, it might have a high activation energy barrier that would slow it down or even prevent it from occurring at a certain temperature.

The second law of thermodynamics asserts that no spontaneous activity ever causes the total entropy of a system to decrease. That is, it may rise or even hold steady, but it never falls. Clearly, the necessity for molecules to be further apart from one another drives all spontaneous activities. How, one would wonder, can entropy be constant? The Gibbs free energy formula suggests that this occurs when the temperature is 0 Kelvin.

$$S_A = \sum_{i=1}^{n} p_i f(p_i)$$

$$S_B = \sum_{j=1}^{m} p_j f(p_j)$$

$$S_C = \sum_{i=1}^{n} \sum_{j=1}^{m} p_{ij} f(p_{ij}) = \sum_{i=1}^{n} p_i f(p_i) \sum_{j=1}^{m} p_j f(p_j).$$

Understanding how quantum theory affects the argument has led to sometimes unexpected statements being made because of the complicated interaction between measurement, irreversibility, and quantum theory.

When explaining the irreversibility of wavefunction collapse on measurement, Von Neumann expressly cited Szilard's theory, but it is unclear exactly what purpose this served. Both Gabor and Brillouin's methods of measuring light required the electromagnetic field to be quantized in order to cause dissipation. Gabor made it very apparent that he believed that measurements made using conventional electromagnetic fields could occur non-dissipatively and result in unrestrained violations of Newton's second law. According to the Landauer-Penrose-Bennett argument, heat is not produced by measurements; therefore, classical statistical mechanics need not result in untamable demons. The fact that some physical processes for measurement disperse heat does not disprove Bennett's argument that other physical processes can perform measurements non-dissipatively, even though it is still possible to argue that quantum electrodynamics dissipates heat if utilized for measurement.[19,20]

Nevertheless, wavefunction collapse and thermodynamic irreversibility are usually linked. There may appear to be a contradiction here because, according to quantum theory, measurement should increase entropy while, according to the Szilard engine, it should potentially lead to a drop in entropy. Alternately, one may consider whether the gain in entropy caused by wavefunction collapse cancels out the loss caused by measurement. These ideas are mostly just confusion, which is simple to fix. Unless the observable being measured commutes with the density matrix, in which case the measurement would leave the Gibbs-von Neumann entropy of the density matrix constant, a projective von Neumann measurement will increase the density matrix's Gibbs-von Neumann entropy.[21,22] However, this also holds true for the density matrix that illustrates the statistical distribution of all measurement results. Even yet, the ensemble spanning all measurement outcomes can nonetheless have a smaller Gibbs-von Neumann entropy than the subensemble density matrix that corresponds to a specific outcome having occurred.

A similar issue regarding the connection between knowledge and thermodynamic entropy appears to be raised by both the Szilard engine and Landauer's principle: if one knew which side of the engine the molecule was on, one could extract work; if one knew which logical state the device was in, one could set it to zero without working. Without this information, it is essential to create a process that operates regardless of the particular state the system is in. However, it is obvious that this does not mean that it is impossible to devise a clever process that can still extract work from an engine without compensation or a clever process that can still reset a bit without labor, even in the absence of information.[23,24] A significant, if mostly overlooked, influence appears to be played by Hamiltonian mechanics and Liouville's Theorem. Non-Hamiltonian flows definitely allow for unrestrained violations of the second law, as Zhang and Zhang's Demon shows, and neither information theory nor computing seem to be able to prevent this.[25,26]

An essential greenhouse gas that aids in keeping heat in our atmosphere is carbon dioxide. Our earth would be uninhabitable cold without it. However, a rise in average global temperatures brought on by rising CO2 levels in our atmosphere is affecting other facets of Earth's climate. Due of CCUS's significance in today's society, CCUS research is rapidly expanding. However, the majority of study is based on CO2 gas phase changes. One of the most crucial foundational sciences for process development in the chemical industry is phase equilibrium thermodynamics. The development of thermal separation processes has undergone a significant change as a result of the exceptional outcomes that thermodynamics has produced over the past several decades.

So, in this work, the entropy details of the CO2 gas at various pressure and temperature conditions is discussed.

2. Methodology

Since CO2's physical qualities differ greatly from those of natural gas and are greatly impacted by temperature, pressure, and pollutants, transporting it requires a phase transition. It's also important to consider the CO2 contamination limit. But, the entropy plays a major role in transforming the CO2 into various physical and chemical forms.

The sample fluid under consideration must be configured using the fluid management interface. The CO2 gas, for which the enthalpy is being estimated, serves as the study's sample fluid. As a result, the defined gas mol percent is selected, and the PVTsim's sample fluid function's fluid management system is turned on. This mole percentage will be 100 because the chosen gas sample is pure gas. To ensure that the gas system is being simulated as a full system, the system is normalized after the concentration has been determined. These details are shown in Figures 1 and 2. The simulations tab is then opened, and the property generator function is chosen. In Figure 3, it can be observed. The property generator toolbox is then prompted, and Figure 4 shows how it appears. It can be seen that a chosen gas or liquid can be obtained with this many qualities for a variety of settings. Therefore, entropy is chosen as the attribute to be evaluated in this study, and the PT specifications are chosen to be single-point calculations because the simulation will be simpler to calculate one point at a time. As the pressure varies in this work while keeping the temperature constant, the output format was chosen as the constant temperature. The water characteristics are thought to be consistent with SRK-EOS. The simulations are then run after entering the pressure information.

In this work, based on the critical pressure, a range of pressure is chosen with an interval of 5 bar. The temperature setting considered for each set of simulation runs was considered as 0,1,2,3 °C.

3. Results & Discussion

The results of the entropy are presented in Table – 1. Representation of the variation of the entropy with respect to change in pressure at a fixed temperature (0°C) is shown in Figure – 3. From these results it can be observed that the increase in pressure is causing the increase in entropy as well. Entropy strongly depends on both pressure and temperature. Because of the rotational, translational, and vibrational motion of the molecules, the system has internal energy. The temperature has a significant impact on internal energy. The relationship between pressure and gas temperature is straightforward. During a phase change, both are dependent on the region of the vapour-liquid mixture. Intermolecular forces will be higher in materials that have been squeezed more. The intermolecular force of solids is greater than that of liquids, which in turn is greater than that of gas.

Similarly, the results at Temperatures 1,2,3°C. Results were found to be the same at any given constant temperature condition. But from the results, presented in Table 1,2,3,4, the change in entropy of the system with the increase in temperature is very negligible. So, the entropy is mostly depending on the pressure of the gas system.

Since the recognized standards of proof and motivations vary greatly across the literature, it can occasionally be challenging to identify any coherent body of work. Maxwell's initial goal was to show that the second law had certain limitations and that there could be violations. He initially spoke of the demon as a living being, but later reduced its function to that of a valve. Smoluchowski created a modified version of the second law that the demon did not breach in an effort to subdue it. Only mechanical devices were subject to his exorcism, and he left open the possibility of intellectual intervention overturning the second law. The exorcism's scope and the demon's characteristics altered as the literature evolved. Information processing carried out by a mechanical device came to represent intelligence. The goal changed from figuring out how a tamed demon might be limited by physical rules to completely excluding demons. A large portion of the resulting literature proceeds case-by-case, arguing that particular demons fail and then extrapolating that all demons would fail for the same reasons.

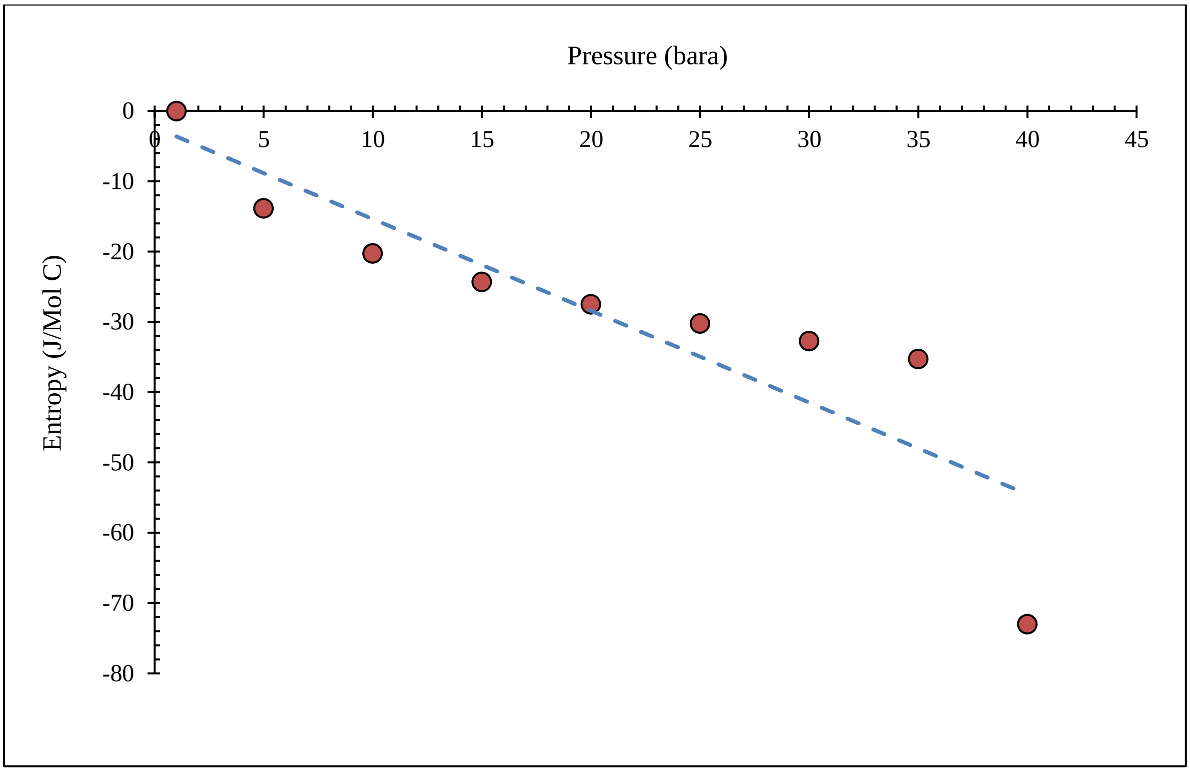

Figure 3: Pressure vs Entropy at 0°C

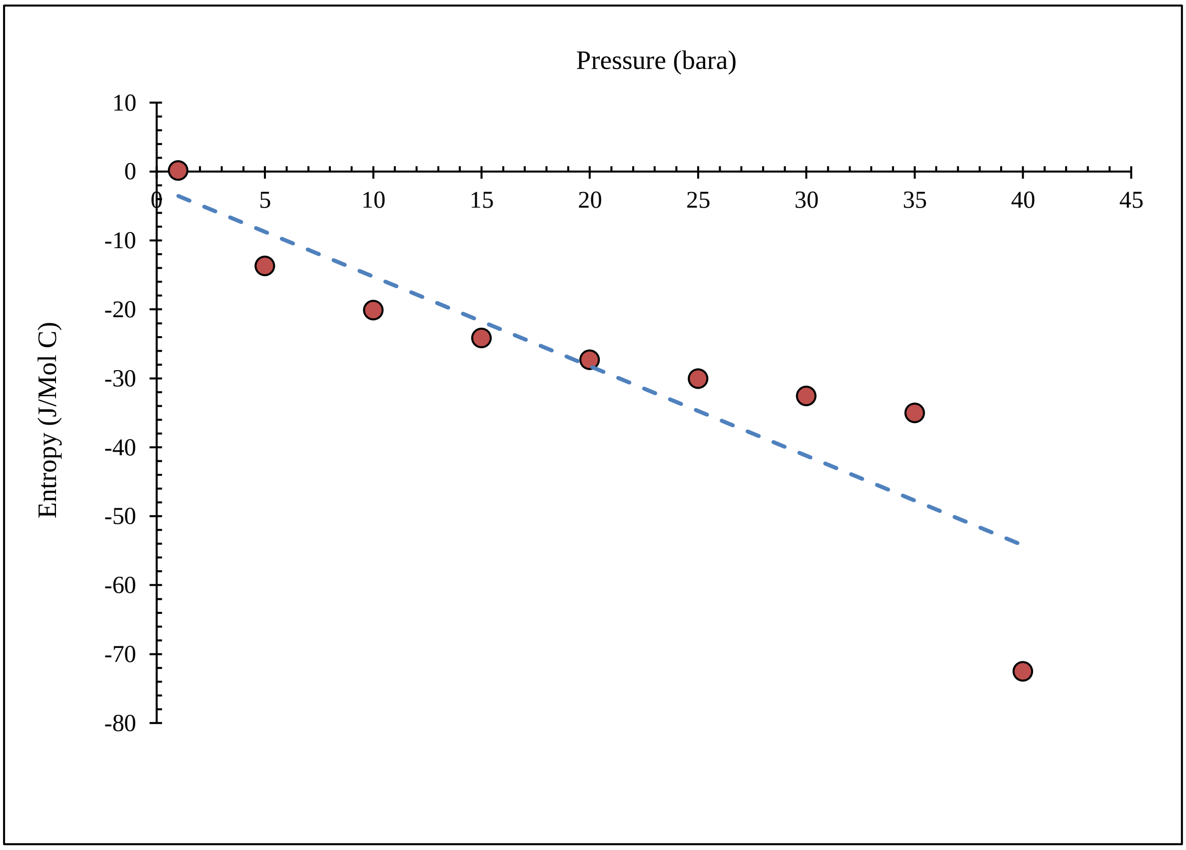

Figure 4: Pressure vs Entropy at 1°C

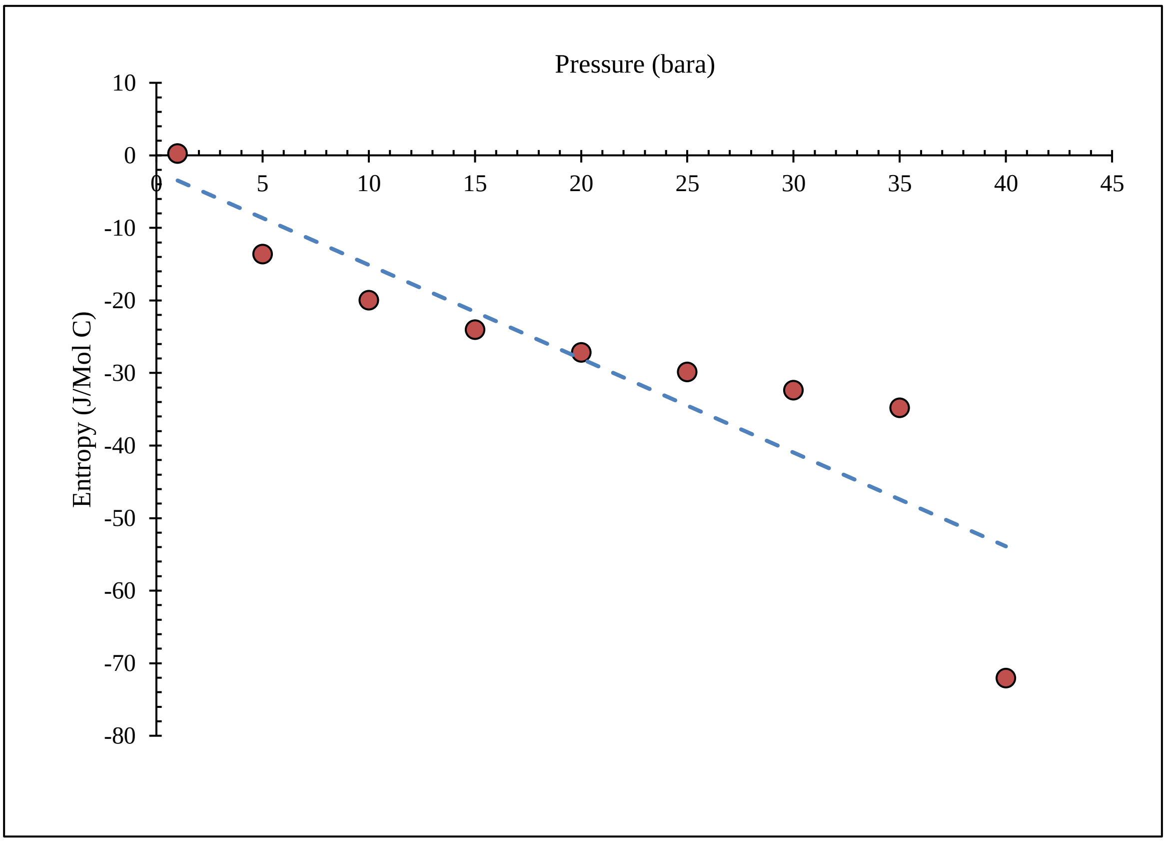

Figure 5: Pressure vs Entropy at 2°C

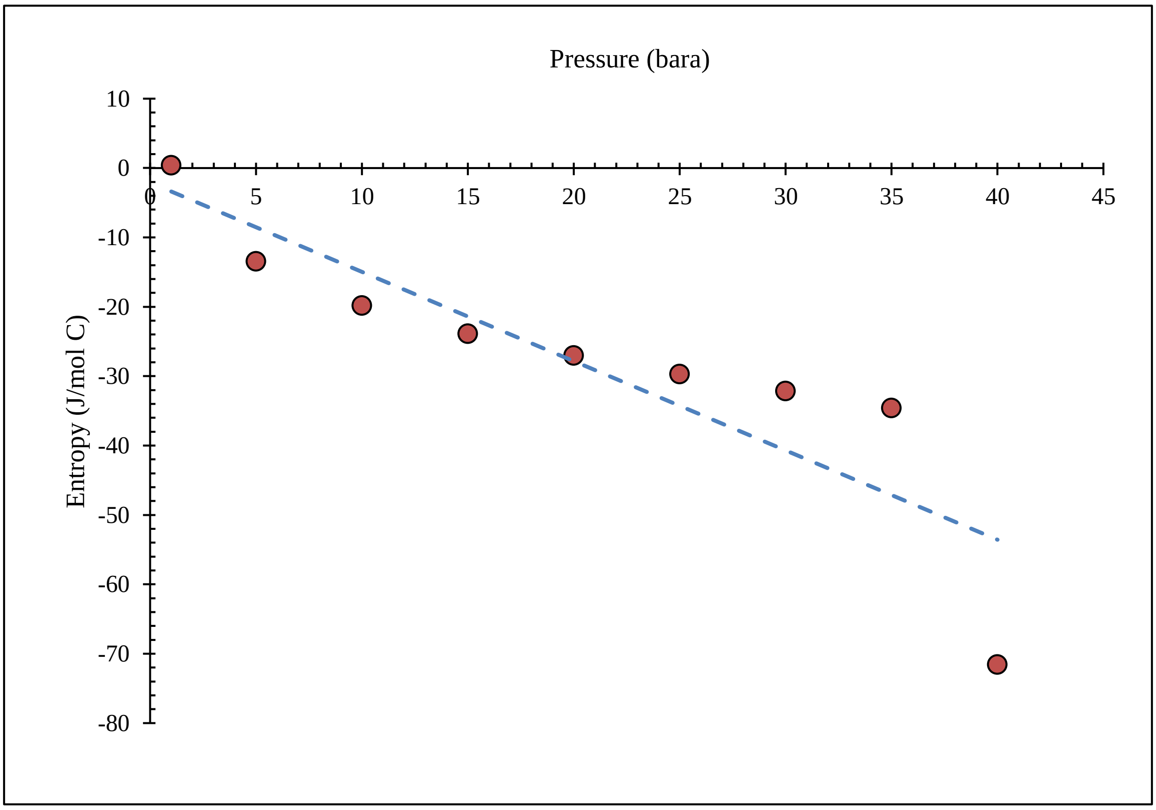

Figure 6: Pressure vs Entropy at 3°C

Table 1. Total Entropy at 0°C

Gas Sample	**S.No**	**P (bara)**	**T (°C)**	**Enthalpy (J/mol)**
CO_2	1	1	0	-0.01
	2	5	0	-13.86
	3	10	0	-20.26
	4	15	0	-24.33
	5	20	0	-27.5
	6	25	0	-30.22
	7	30	0	-32.75
	8	35	0	-35.27
	9	40	0	-72.99

Table 2. Total Entropy at 1°C

Gas Sample	**S.No**	**P (bara)**	**T (°C)**	**Enthalpy (J/mol)**
CO_2	1	1	1	0.13
	2	5	1	-13.73
	3	10	1	-20.12
	4	15	1	-24.18
	5	20	1	-27.33
	6	25	1	-30.05
	7	30	1	-32.56
	8	35	1	-35.04
	9	40	1	-72.52

Table 3. Total Entropy at 2°C

Gas Sample	**S.No**	**P (bara)**	**T (°C)**	**Enthalpy (J/mol)**
CO_2	1	1	2	0.26
	2	5	2	-13.59
	3	10	2	-19.98
	4	15	2	-24.03
	5	20	2	-27.17
	6	25	2	-29.87
	7	30	2	-32.36
	8	35	2	-34.81
	9	40	2	-72.04

Table 4. Total Entropy at 3°C

Gas Sample	S.No	P (bara)	T (°C)	Enthalpy (J/mol)
CO_2	1	1	3	0.39
	2	5	3	-13.45
	3	10	3	-19.83
	4	15	3	-23.88
	5	20	3	-27.01
	6	25	3	-29.7
	7	30	3	-32.17
	8	35	3	-34.58
	9	40	3	-71.55

4. Conclusion

The amount of thermal energy per unit of temperature in a system that cannot be used to carry out beneficial work is known as entropy. Entropy is a measure of a system's molecular disorder or unpredictability since work is produced by organized molecular motion. It aids in figuring out an object's thermodynamic condition. A little thought will reveal that a spontaneous process shifts from a less probable condition to a more probable state when it occurs. It expresses the condition of a body in the same way as temperature, pressure, volume, internal energy, and magnetic behaviour. So, in this work, the entropy details of the CO2 gas at various pressure and temperature conditions are discussed. It was observed that the entropy of the system is highly dependent on the pressure of the gas in a closed system. Also, the entropy is directly proportional to the pressure of the gas.

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