National University of Sciences and Technology (NUST)
School of Electrical Engineering and Computer Science

ME – 102: Thermodynamics

Instructions: Late submissions will not be accepted.
Date of Submission: Tuesday, December 7th, 2021 (after the lecture)

1. You can make a **Group of two persons** for doing this assignment
2. Length of submission must not be more than **2 A-4 Pages (Double Sided, Font Size 11, Arial/Calibri Font, 1.0 line spacing)**,
3. Zero tolerance to plagiarism
4. Five marks for neat & clean submission, and originality certificate attached with the assignment.

Use your knowledge of Thermodynamics to briefly discuss* its aspect in.

i) **Biological Systems**
ii) **Nanotechnology**

***Discussion must cover the technical / computational / experimental point-of-view.**

Group Members

Name	CMS ID	Topic
Muhammad Ahmed Mohsin	333060	Biological Systems
Muhammad Umer	345834	Nanotechnology

Biological Systems & Thermodynamics

Abstract

Thermodynamics deals with the study of heat flow through different systems in different conditions. Biological thermodynamics deals with energy transductions within living organisms. Thermodynamics plays an important role in studying the functioning of different chemical processes that take place within these systems.

Technical Point of View

Energy Transformation

Energy transformation taking place within our systems are determined with the help of thermodynamics. Sun is the most important form of energy for living organisms and the formula that determines the wavelength and frequency for this energy is given by:

$$E = \frac{hc}{\lambda} = h\nu$$

Hess Law and Calorimeter

Hess law states that the heat entering and leaving a reaction is equal. This is the basis for the calorimeter which is used to determine amount of heat in a chemical reaction. As the heat enters a biological system in oxidized form the production is estimated using calorimeter in kilojoules.

Gibbs Free Energy

Gibbs law in thermodynamics develops an inter relation with biological reactions. It states that energy and entropy change simultaneously. It can be used to determine a reaction occurring spontaneously. For example, the reaction between glucose and fructose to sucrose occurs spontaneously with *+5.5 k mole/cal*. If the energy is negative, then it won't occur spontaneously.

Experimental Point of View

Bioengineering Of Thermodynamics of Cells

Cells are complex thermodynamics systems. They are regarded as complex engines to run different thermo-electrical-chemical processes. Different thermo-biochemical behaviors occur between health and disease states. The heat is dissipated into the environment which can be a new approach to study the behavior of cells and control their behavior. The total entropy of the closed biological system dissipating heat in disease state is given by:

$$dS = d_i S + d_e S$$

The analysis of this new approach concludes that cell behaviors are based on the ion fluxes across the cell membranes.

Separation of Time Scales in Thermo-Biological Systems

For thinking about the processes in the living world one the constraint is the assumption of fixed temperature, and this is equivalent to imposing the constant mean energy. This assumption is mostly true because the temperature changes are very slow in nearly all biological systems. On the other hand, if we want to consider the disposition of DNA molecule on a surface then we consider very rapid heat changes. This application of time scale change can simplify many tasks if the temperature is constant.

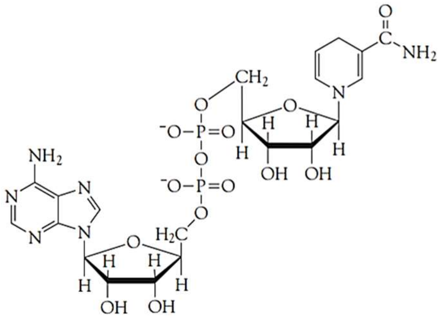
Thermodynamic Models of Binding

One of the important aspect of thermodynamics is its usefulness in the study of biological binding reactions. By determining the binding energies and molecular enthalpy of chemical reactions within the organisms it can be determined about the prediction od binding of molecules in the bio-chemical reactions as well. Thermodynamics can be used to predict he feasibility of the chemical reactions.

Computational Point of View

Energy Conservation in Living Organisms

The processes taking place inside the biological systems such as metabolism and catabolism are either endothermic or exothermic.



3 NADH

The above shows a highly exothermic reaction. Thermodynamics is used in computational aspect of calculation of enthalpies of reactions.

Numerical Example

Problem Statement

Exhalation of air during breathing requires work because air must be pushed out from the lungs against atmospheric pressure. Consider the work of exhaling 0.50 L (5.0×10^4 m3) of air, a typical value for a healthy adult, through a tube into the bottom of the apparatus and against an atmospheric pressure of 1.00 atm (101 kPa). The exhaled air lifts the piston so the change in volume is V = 5.0×10^4 m3 and the external pressure is p_{ex} = 101 kPa.

Solution

The work of exhaling is given by:

$$
\begin{aligned}
w &= -p_{ex} \nabla V \\
&= -(1.01 \times 10^5 \; Pa) \times (5.0 \times 10^{-4} m^3) \\
&= -51 \; Pa \, m^3 \\
&= \boldsymbol{-51 \; J}
\end{aligned}
$$

Where we have considered 1 Pa m^3 = 1 J.

ATP Cycle and Reaction Coupling

The most significant application of thermodynamics is around ATP and energy consumption rate which is an important parameter for modelling energy demands for cell growth.

The hydrolysis of ATP through water mediated breakdown Is also studied under thermo-biological reactions.

$$\mathrm{ATP} + \mathrm{H_2O} \leftrightharpoons \mathrm{ADP} + \mathrm{P}_i + \mathrm{energy}$$

Reaction coupling is given by:

$$
\begin{array}{ll}
\mathrm{A} \leftrightharpoons \mathrm{B} & \Delta G = X \\
+\,\mathrm{B} \leftrightharpoons \mathrm{C} + \mathrm{D} & \Delta G = Y \\
\hline
\mathrm{A} \leftrightharpoons \mathrm{C} + \mathrm{D} & \Delta G = X + Y
\end{array}
$$

Applications

Other applications of thermodynamics in biological systems include:

- Metabolism and Catabolism
- Sweating from Body
- Changes in Cell behavior during diseases due to temperature
- Travelling of energy in oxidized form throughout the body

These are some of the many applications of thermodynamics in biological systems.

Conclusion

Thermodynamics plays a vital role in determining the physical processes going on within the living bodies. From heat of enthalpies to physical binding of molecules everything can be predicted with the help of thermodynamics. Moreover, with the help of thermodynamics different physical applications are made such as calorimeter which are used in different places. In a nutshell everything involves thermodynamics.

Nanotechnology & Thermodynamics

Abstract

Nanotechnology is expected to significantly affect long-term development within and across many disciplines. However, when working with materials and particles at a much smaller scale, it becomes a challenge to keep unavoidable processes in – check and for that purpose we study the effects of thermodynamics on such a scale extensively, under a collective term of nanothermodynamics. This report aims to get a brief overview of the applications in which thermodynamics is extensively utilized and discuss their technical, experimental, and computational aspects.

Introduction

The laws and principles of thermodynamics find applications in almost all the sectors of science and engineering. Although the classical thermodynamics laws uphold universally, however, they prove to be insufficient when dealing with the likes of genetics, microfluids, and nanoparticles, etc.

The primary premise of nanothermodynamics, as put forth by T. L. Hill, is that a large collection of subsystems must behave and act as a large system. Thus, nanothermodynamics serves as a bridge between the macro and microscopic thermal properties.

Different Approaches to Nanothermodynamics

An overview of two of the most famous approaches to nanothermodynamics are discussed in this section:

Hill's Theory

Hill introduced a new thermodynamic potential by conceptualizing finite size effects within the macroscopic thermodynamics called the sub-division potential, U_{sub}, and it is defined as:

$$\boldsymbol{U_{sub}} = \left(\frac{\boldsymbol{\partial U}}{\boldsymbol{\partial N_{sub}}}\right)_{S,V,N}$$

Where: *U is the internal energy, S is the entropy, V is the volume, N is the number of particles, N_{sub} is the number of sub-divisions*

Fundamentally, the sub-division potential, U_{sub}, denotes the change in required to take *N* interacting particles from a bath of clusters into the system.

Tsallis' Theory

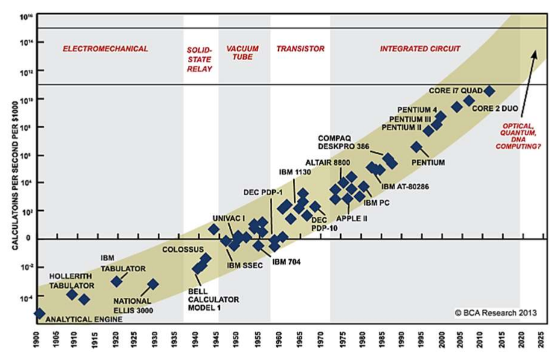
Unlike Hill's theory, the Tsallis' approach aims to redefine entropy by considering the non – extensivity of small systems, rather than redefining internal energy *U*. The mathematics involved with this approach is too complex for the scope of this report.

Practical Utilization of Nanothermodynamics

We shall only look at those applications of Nanothermodynamics that is both related to what has been discussed above as well as how relevant it is to the authors of this report, that is, university students.

Microprocessors

An observatory law presented by Gordon E. Moore in 1956, states that *the number of transistors on a microchip double about every two years, though the cost of computers is halved.*



Moore's Law

Presently, transistors in microprocessors reaching 10 – 3 nm in size, at this scale, traditional power dissipation methods, i.e., using copper heatsinks, delidding the chip, etc. fail to cool the ensemble down. The total power consumption of a CPU via logical activity of transistors is given by:

$$P_{cpu} = P_{dyn} + P_{sc} + P_{leak}$$

Cooling a microprocessor at this scale, becomes an extensive application of thermodynamics and poses a major challenge to the future of computation. This cooling demand may be represented as:

$$(T_j - T_a)/\mathrm{TDP}$$

Which is the required thermal resistance of the die

Thermal management is arguably the biggest technical as well as an economic challenge in the fabrication of transistors. These thermal solutions are then faced with the problem of cost and is often the reason why newer technologies may find barriers to introduction particularly if it cannot supplant an existing product on a cost – efficiency basis. Collectively, all these factors are dealt with and under the study of Thermodynamics.

Nanothermodynamic Properties of Ferromagnetic Nanoclusters

Nanostructural materials, compared to ordinary materials have much preferable and sophisticated thermal properties. The mean energy for each particle in such a cluster is given as:

$$\varepsilon(H,L,N) = -\bar{h}\left(\frac{2L}{N}-1\right) - \frac{CJ}{2}\left[\frac{4L(L-1)}{N(N-1)} - \frac{4L}{N} + 1\right]$$

$\bar{h}$ here represents the magnetic permeability of vacuum.

$$\bar{h} = \mu_0 \mu_m H$$

For this partition function, we can find the total thermodynamic properties as follows:

$$U(H,L,N)$$
$$S(H,L,N) = k_\beta \ln\left(Z(T,N)\right)$$

From observation, we can see that both the internal energy and the total entropy of this system depends solely on the magnetic intensity H, number of particles in up – state L, and the number of clusters N. Using the mean – field theory, we provide ourselves with canonical partition functions leading to variations of Gibbs and Helmholtz free energies in terms of Temperature T.

This energy plays an important role in dividing a big system into smaller pieces. Furthermore, thermodynamics play a dire role in the computational aspect of this analysis and the applications of ferromagnetic materials on an industrial level are ever expanding.

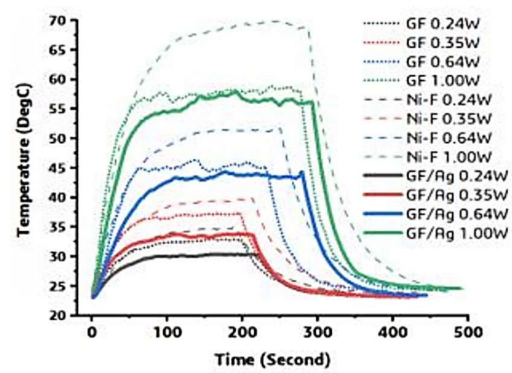
Low Temperature Sintering

Sintering is defined as the collective result of thermally activated atomic level processes through diffusion, creep, plastic and viscous flow and evaporation. The following expression the most common model for the sintering of free particles:

$$\sigma = \gamma . \left[\frac{1}{R_1} - \frac{1}{R_2}\right]$$

Where:
σ: driving force
γ: material surface energy
R_1 and R_2: principal radii of curvature and can be function of concave or convex surfaces

These sintering processes are then further utilized in synthesis of graphene which is arguably the forefront of nanotechnological innovation. Thermal properties of graphene and its reaction with metals allow for it to be a great tool in electronics. A foam coated heat sink produced from this nanostructure acts as a great thermal dissipator and is in continuation with the discussion we left off in microprocessors; to effectively cool the thermal output while achieving greater performance ignoring the past limitations.



This graph displays and abstracts thermal cooling properties of graphene foam with respect to other modern day heat sinks.

Conclusion

Thermodynamics acts as a keystone of development in every scientific research and discovery. Going from the macro – scale to the nano – scale, there is, however, a transition from exponential laws describing a continuous material to power laws describing a discrete material. The appearance of those power laws is the result of strong correlations between the physio-chemical properties with the size, shape, and environment of the nanoparticle.

This report discussed some of the many of advanced applications, as well as foundational theories and laws, of nanothermodynamics, while giving a brief overview of said topics, in order to elucidate the role of thermodynamics in our lives, and scientific discoveries as a whole.