



Research Paper

Modelling the dependency of a non-steady diffusion on temperature of a conductive material

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ABSTRACT

The concentration of a diffusing species is a function of both time and position, $u = u(x, t)$. The species used in this study was a copper which was allowed to diffuse into a bar of copper (a host metal). The analytic method was used to establish the concentration of the material with the independent variables x and t . The effect of temperature on concentration and the thermal diffusivity of a material D were determined using numerical simulation. The results were showed on diverse plots at different temperatures.

Stephen Okeke^{1*}, Damasus Arinze Nworah²,
Jummai Adamu Tutuwa³

¹Department of Mathematics/Statistics, Ignatius
Ajuru University of Education, Port Harcourt,
Nigeria.

^{2,3}Bioresources Development Centre, National
Biotechnology Development Agency, Jalingo,
Taraba State, Nigeria.

*Corresponding author. Email:
oikennastephen@gmail.com

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INTRODUCTION

Temperature has a great effect on the rate of metal electrochemical corrosion. It is the measure of hotness or coldness expressed in terms of any of numerous capricious scales and signifying the direction, in which heat energy will instinctively flow; that is from a hotter body which is one at a higher temperature to a colder body which is one at a lower temperature. An increase or decrease in the temperature of system at equilibrium is a stress to the system. In the Haber-Bosch process, the concentration of NH_3 in the system decreases, as there is an increase in the concentrations of N_2 and H_2 . Thus, an increase in temperature enhances the reverse reaction (endothermic direction). The concentration of NH_3 in the system increases as there is a decrease in the concentration of N_2 and H_2 . Thus, a decrease in temperature enhances the forward reaction. Meetham (1991) showed that in most industries, transportation and power generation occur as a result of high temperature of materials by investigating on the high-temperature aluminum alloys, steels and nickel alloys. Temperature is a measure of the quality of a state of a material. One effect that leads to CO structure involves its formation by passing air over surfeit carbon at high temperature. The early product (carbon dioxide)

equilibrates with the residual hot carbon, resulting to carbon monoxide. CO_2 formation is no-expense-spared at lower temperature whereas CO is the major product above 800°C . The conductance is a measure of how easily those charge particles move through a solution or material usually measured in Siemens, S while the conductivity is the conductance (S) measured across a specified distance through a material or solution usually measured in Siemens per centimeter, S/cm. The activation energy is the energy that must be provided to compounds to result in a chemical reaction. It was introduced in 1889 by the Swedish scientist Svante Arrhenius. His equation gives the quantitative center of the relation between the activation energy and the rate at which a reaction proceeds. Diffusion is a vital aspect of most chemical and biological phenomena. In chemical processes, diffusion is frequently the central principle driving many reactions. For instance, a few crystals of sugar in a glass of water will slowly dissolve over time. This occurs since there is a net movement of sugar molecules into the water medium while in biological systems, diffusion occurs across membranes in every cell as well as through the body. As an example, oxygen is at a higher concentration inside arteries and arterioles, when

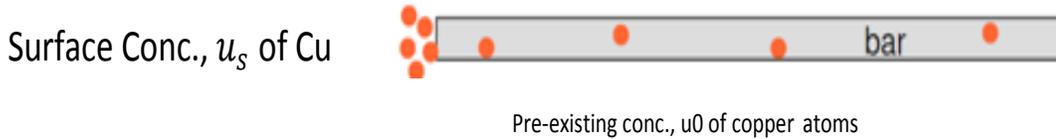


Figure 1: Copper diffuses into a bar of copper.

compared with the oxygen levels in actively respiring cells. There are factors that affect the diffusion; they include: temperature, area of interaction, concentration difference, particle size and diffusing species.

Miao et al. (2014) investigated on the thermo-physical features for four rock types which included the granite, granodiorite, gabbro and gernet amphibolites ranging from room temperature to 1,173K and specific heat capacity using laser-flash method and heat flux differential scanning calorimetry respectively. Their result was that the rock thermal diffusivity and conductivity declined as the temperature increased and approached a constant value at high temperatures.

Wen et al. (2015) carried out a scientific work on the thermal properties of coal and rocks using the laser-flash apparatus LFA457. Their result suggested that the method was able to accurately determine the thermophysical properties for rocks; when the temperature increased, there was a decrease in the thermal diffusivity and thermal conductivity.

In line with Mehrer and Stolwijk (2009), diffusion is a scientific discipline that is based on various cornerstones such as the continuum theory, the Brownian motion, solid-state and atomistics of diffusion in materials which had driven an important contribution to Einstein, Arrhenius, Perrin, von Hevesy and Bardeen. In terms of interdiffusion, atoms tend to migrate from regions of high concentration to regions of low concentration in an alloy. Thus, diffusion is a stepwise migration of atoms from lattice site to lattice site. Hence, a self-diffusion.

This study is interested in modelling the dependency of diffusion on temperature of a conductive material (copper tin rod) which is a metallic material that is an extreme case of the problem imposed by conductivity.

A copper, Cu is a chemical element, a soft, malleable, ductile reddish-brown metal with very high thermal and electrical conductivity with atomic number 29 which is important to plumbing, electrical wiring; living organisms such as in fish and other vertebrates including human which has formed mainly in the liver, muscle and bone. Copper (II) salts are commonly encountered compounds which have been used extensively and in olden times as pigments which also exist in an aqueous solution.

In nature, copper occurs in the aquatic environment in low concentration (Woody and O'Neal, 2012). Nordberg et al. (2007) suggested that seawater copper concentrations are generally less than 1 part per billion (ppb). Davis et al. (2000) suggested that a high aquatic copper concentrations

mainly occurs copper mining and smelting facilities and in developed areas. The said aquatic habitats are subject to copper pollution (Nriagu 1979; Davis et al, 2000); NAS (1977) in Woody and O'Neal (2012) highlighted that the copper is highly lethal to freshwater fish in soft water at low concentration ranging from 10 – 20 ppb.

Scientists such as Gupta et al. (1999), Gomez and Bosecker (1999), Deng et al. (2007) and Green-Ruiz et al. (2008) in Aston et al. (2010) reported an increase in loading capabilities of metals with increasing temperature.

Aston et al. (2010) examined the cause of cell condition, pH and temperature on lead (Pb), zinc and copper sorption to acidithiobacillus caldus strain using Langmuir model. Their result showed that far less copper was improved from viable cells than any other metal or cell state.

MATHEMATICAL FORMATION

Following Okeke and Nwagor (2019) in Philibert (2006), considering the concentration of the diffusant at a point x meters along a bar tin rod at t represented by $u(x, t)$, then a one dimensional heat equation is:

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, 0 \leq x \leq L, t \geq 0. \quad (1)$$

Where $u = u(x, t)$ is the dependent variable, and D is a constant coefficient due to the bar rod material as shown in Figure 1.

Thermal diffusivity measures the rate of transfer of heat of a material from the hot end to the cold end. It is given as $D = \frac{k}{\rho c_p}$, where: k is the thermal conductivity ($\frac{W}{m.K}$), c_p is specific heat capacity ($J/(kg/K)$), ρ is density (kg/m^3) and ρc_p is the volumetric heat capacity ($J/(\frac{K}{m^3})$).

Let D represents the thermal diffusivity of a material, M is the modified frequency factor (pre-exponential factor), Q is the activation energy (J/ mole), R is the universal gas constant (8.314 J/mol-K) and T is the absolute temperature (K), then, following Arrhenius-type plot equation, the effect of temperature and activation parameters for some systems can be estimated as:

$$D = M \text{Exp} \left(-\frac{Q}{RT} \right) \quad (2)$$

The diffusion coefficient, D increases with increasing

Table 1: A Table showing the diffusion data.

Diffusing Species	Host Metal	$D_0(m^2/s)$	Activation Energy Q_d		Calculated Values	
			kJ/mol	$eV/atom$	$T(^{\circ}C)$	$D(m^2/s)$
Fe	α -Fe (BCC)	2.8×10^{-4}	251	2.60	500	3.0×10^{-21}
					900	1.8×10^{-15}
Fe	γ -Fe (FCC)	5.0×10^{-5}	284	2.94	900	1.1×10^{-17}
					1100	7.8×10^{-16}
C	α -Fe	6.2×10^{-7}	80	0.83	500	2.4×10^{-12}
					900	1.7×10^{-10}
C	γ -Fe	2.3×10^{-5}	148	1.53	900	5.9×10^{-12}
					1100	5.3×10^{-11}
Cu	Cu	7.8×10^{-5}	211	2.19	500	4.2×10^{-19}
Zn	Cu	2.4×10^{-5}	189	1.96	500	4.0×10^{-18}
Al	Al	2.3×10^{-4}	144	1.49	500	4.2×10^{-14}
Cu	Al	6.5×10^{-5}	136	1.41	500	4.1×10^{-14}
Mg	Al	1.2×10^{-4}	131	1.35	500	1.9×10^{-13}
Cu	Ni	2.7×10^{-5}	256	2.65	500	1.3×10^{-22}

Source: E. A. Brandes and G. B. Book (Editors), Smithells Reference Book, 7th edition, Butterworth-Heinemann. Oxford, 1992.

temperature, T.

In a linear form, equation (2) can be written as:

$$\ln D = \ln M - \frac{Q}{RT} \tag{3}$$

For two thermal diffusivities at two different temperatures, equation (3) leads to (4) and (5):

$$\ln D_1 = \ln M - \frac{Q}{RT_1} \tag{4}$$

$$\ln D_2 = \ln M - \frac{Q}{RT_2} \tag{5}$$

$$(5) - (4): \ln D_2 - \ln D_1 = \ln M - \frac{Q}{RT_2} - \ln M + \frac{Q}{RT_1}$$

This implies that $\ln D_2 - \ln D_1 = -\frac{Q}{RT_2} + \frac{Q}{RT_1}$, so that:

$$\ln D_2 - \ln D_1 = \frac{Q}{RT_1} - \frac{Q}{RT_2}$$

$$\ln \frac{D_2}{D_1} = \frac{Q}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \tag{6}$$

$$2.303R \log \frac{D_2}{D_1} = Q \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \tag{7}$$

This last equation becomes: $\log \frac{D_2}{D_1} = \frac{Q}{2.303R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$ (8)

This implies that from (3): $\ln D - \ln M = -\frac{Q}{RT}$. (9)

Thus from (9), as $T \longrightarrow \infty, D \longrightarrow M$

Solving equation (1) using separation of variable to get:

$$u(x, t) = Ce^{-Dk^2t} (c_1 \cos kx + c_2 \sin kx) \tag{10}$$

This implies that, $u(x, t) = Ce^{-k^2Dt} (\cos kx + \sin kx)$ (11)

Hence, $(x, t) = Ce^{-k^2t} \exp\left(-\frac{Q}{RT}\right) (\cos kx + \sin kx) : c_1 = c_2 = 1$. (12)

Where C is the constant formed from integrating process in the absolute temperature.

RESULTS AND DISCUSSION

The results are presented below with examined simulated data. From Table 1 for the diffusing species (Cu) to the host metal (Cu), the temperatures 873K, 973K, 1073K, 1173K and 1273K with their corresponding diffusion coefficients are gotten from (6).

Thus:

$$D_2 = D_1 e^{\left[\frac{Q}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right]} \tag{13}$$

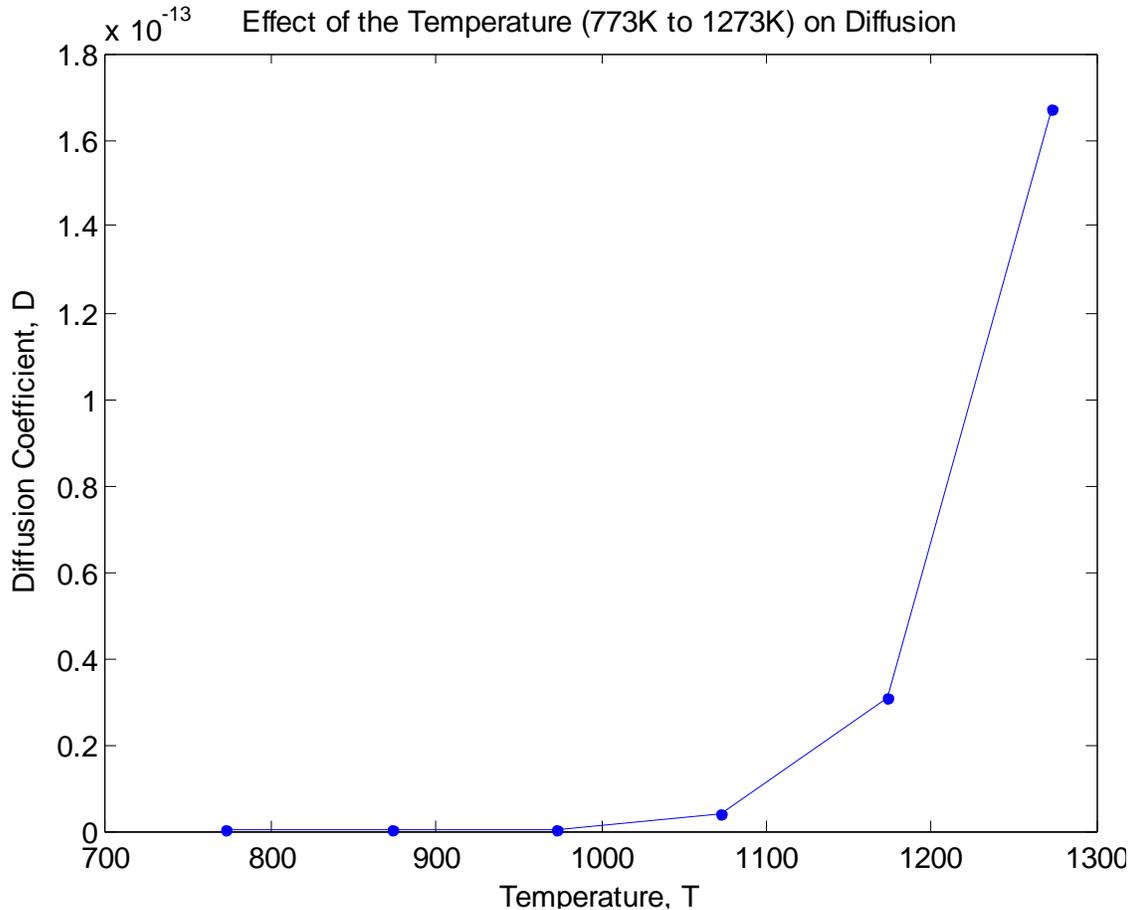


Figure 2: A Graph showing the effect of the temperature from 773k-1273k.

Table 2: A Table showing the calculated diffusion data for the temperature 773K-1273K.

Temperature (K)	Diffusion Coefficient (m ² /s)
873	1.8053e-017
973	3.5818e-016
1073	4.0721e-015
1173	3.0586e-014
1273	1.6736e-013

The equation (13) helps to formulate the diffusion coefficients at the different temperatures (773K – 1273K). The plot for the simulated data above is shown in Figure 2 below. The plot for linearization for the Table 2 is shown in Figure 3 below.

With help of equation (13), Table 3 is formed. The plot for the simulated data above is shown in Figure 4 below. The plot for ln (D) against 1/T for the Table.3 is shown in Figure 5 below. The plot for the simulated data in Table 4 is

shown in Figure 6 below. The plot for linearization for the Table 4 is shown in Figure 7 below.

From (1), as $L \rightarrow \infty$: the following boundary conditions (B.C) for an infinite slab (a tin bar rod) are obtained.

Boundary Condition:

at $t = 0, u = u_0$ for $0 \leq x \leq \infty$, and at $t > 0, u = u_s$ for $x = 0$ (a constant surface concentration)

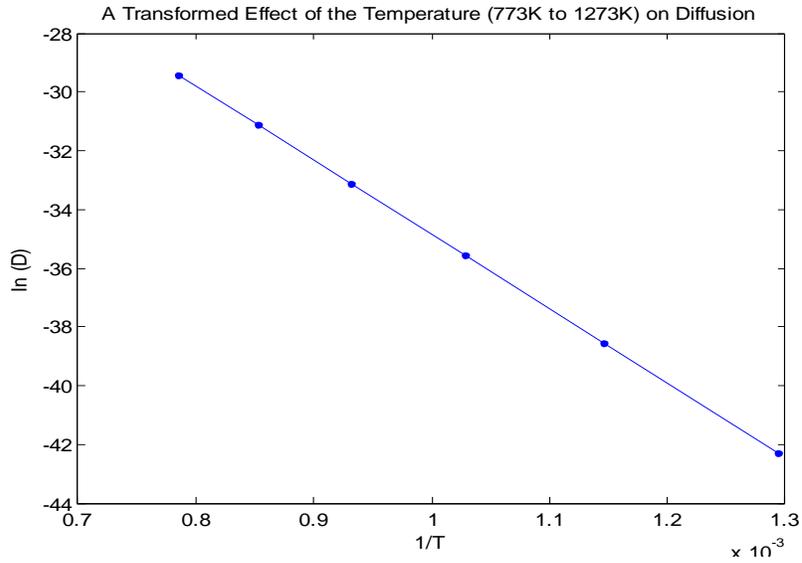


Figure 3: A graph showing a transformed effect of the temperature from 773k-1273k.

Table 3: A Table showing the calculated diffusion data for the temperature 773k-1128k.

Temperature (K)	Diffusion Coefficient (m ² /s)
784	1.4018e-019
843	6.4156e-018
938	1.3534e-016
1033	1.6295e-015
1128	1.2902e-014

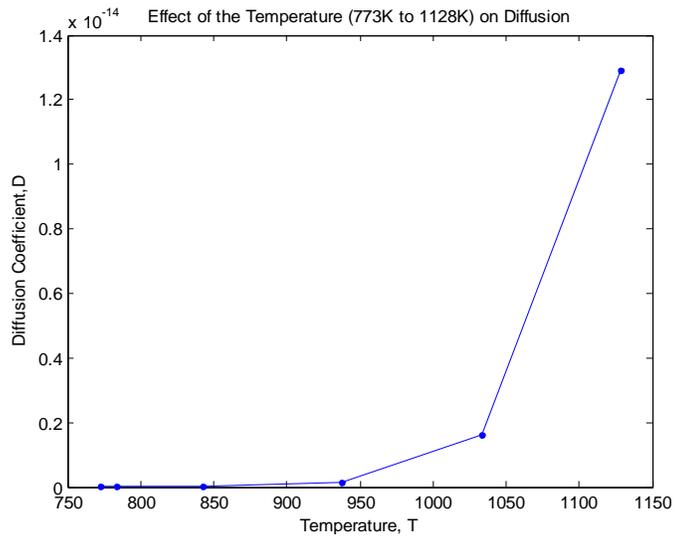


Figure 4: A graph showing the effect of the temperature from 773k-1128k.

for $t_{j+1} > t_j > 0: j = 1,2,3, \dots$

$u = u_0$ for $x = \infty$

(14)

The solution u can be interpreted (Atkinson et al., 2009) as the concentration of the diffusing species at position x and time t . The assumption made here was that there is

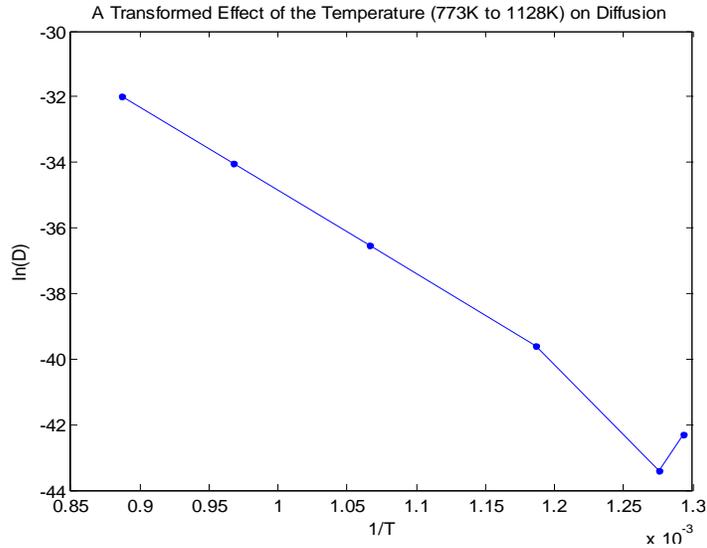


Figure 5: A graph showing a transformed effect of the temperature from 773k-1128k.

Table 4: A Table showing the calculated diffusion data for the temperature 773k-4773k.

Temperature (K)	Diffusion Coefficient (m ² /s)
2773	8.0749e-009
3273	3.2684e-008
3773	9.1328e-008
4273	2.0065e-007
4773	3.7380e-007

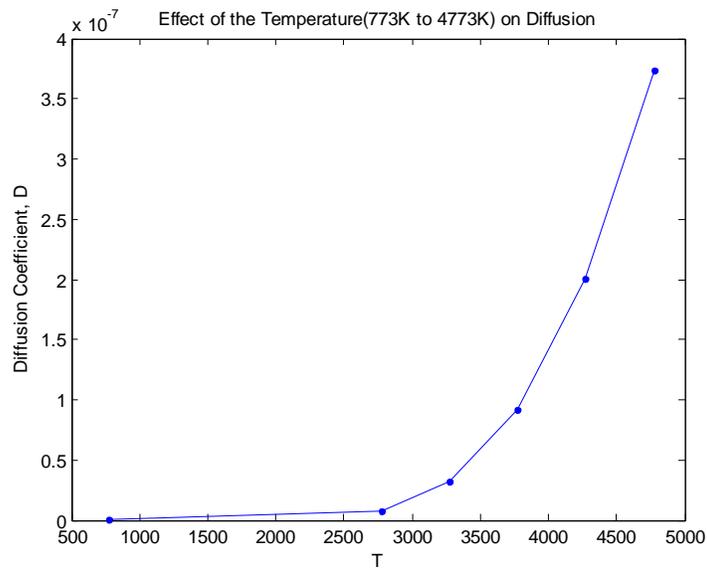


Figure 6: A graph showing the effect of the temperature from 773K-4773K.

negligible resistance to mass transfer at the surface of the object.

One important solution to equation (1) for the semi-infinite solid (a tin bar rod) is:

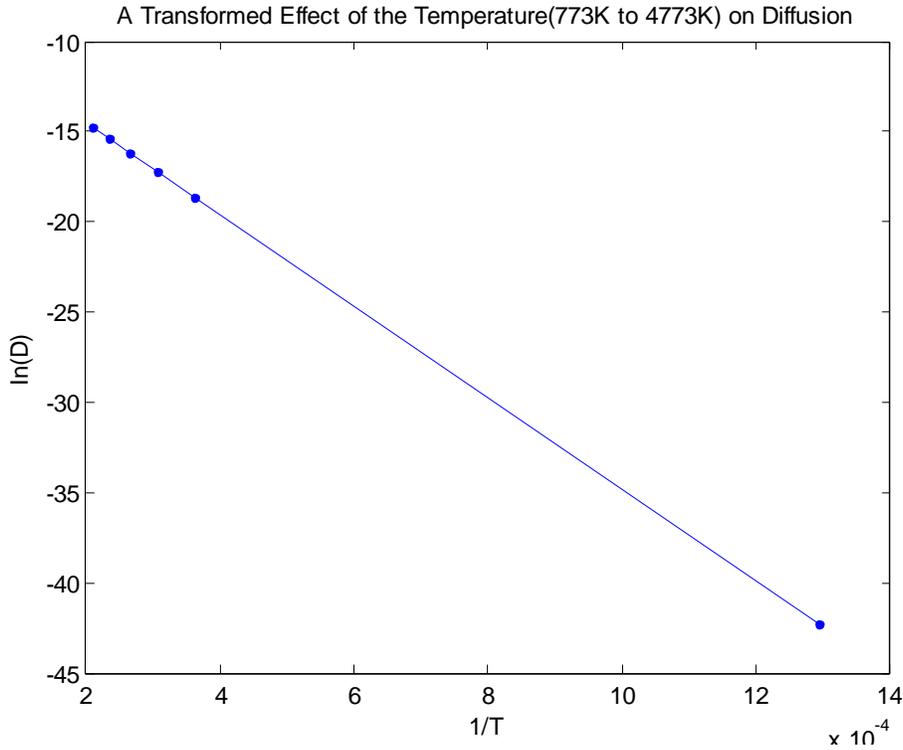


Figure 7: A graph showing a transformed effect of the temperature from 773K-4773K.

Table 5: Table showing the error function values.

z	$erf(z)$	z	$erf(z)$	z	$erf(z)$
0	0	0.55	0.5633	1.3	0.9340
0.025	0.0282	0.60	0.6039	1.4	0.9523
0.05	0.0564	0.65	0.6420	1.5	0.9661
0.10	0.1125	0.70	0.6778	1.6	0.9763
0.15	0.1680	0.75	0.7112	1.7	0.9838
0.20	0.2227	0.80	0.7421	1.8	0.9891
0.25	0.2763	0.85	0.7707	1.9	0.9928
0.30	0.3286	0.90	0.7970	2.0	0.9953
0.35	0.3794	0.95	0.8209	2.2	0.9981
0.40	0.4284	1.0	0.8427	2.4	0.9993
0.45	0.4755	1.1	0.8802	2.6	0.9998
0.50	0.5205	1.2	0.9103	2.8	0.9999

$$\frac{u(x,t)-u_0}{u_s-u_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{15}$$

Where u_x or $u(x,t)$ = concentration at x , u_0 = initial concentration of species at $t = 0$, u_s = surface concentration of species at $x = 0$.

$\operatorname{erf}(x)$ = error function = $\frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy$, whose values are given in Table 5 above. Interpolation is used to determine

any value between values of two entries in the Table 5. The formula below simplifies it.

$$\operatorname{Erf}(z) = \frac{z-z_0}{z_1-z_0} [\operatorname{erf}(z_1) - \operatorname{erf}(z_0)] + \operatorname{erf}(z_0) \tag{16}$$

Illustrated Example 1: Considering a diffusing species (Cu) into a host pure metal (Cu) with the examined

Table 6: A Table showing the simulated data from illustrated example 1.

x(m)	t(seconds)	T(K)	D	erf(z)	u(x,t)
0.002	50	773	4.2×10^{-19}	1.000	0.00
0.004	100	2773	8.0749e-009	0.9984	3.292590385972627e-004
0.006	150	3273	3.2684e-008	0.944650355492137	0.011069928901573
0.008	200	3773	9.1328e-008	0.814365350124814	0.037126929975037
0.010	250	4273	2.0065e-007	0.681904363116498	0.063619127376700
0.012	300	4773	3.7380e-007	0.577032216225337	0.084593556754933

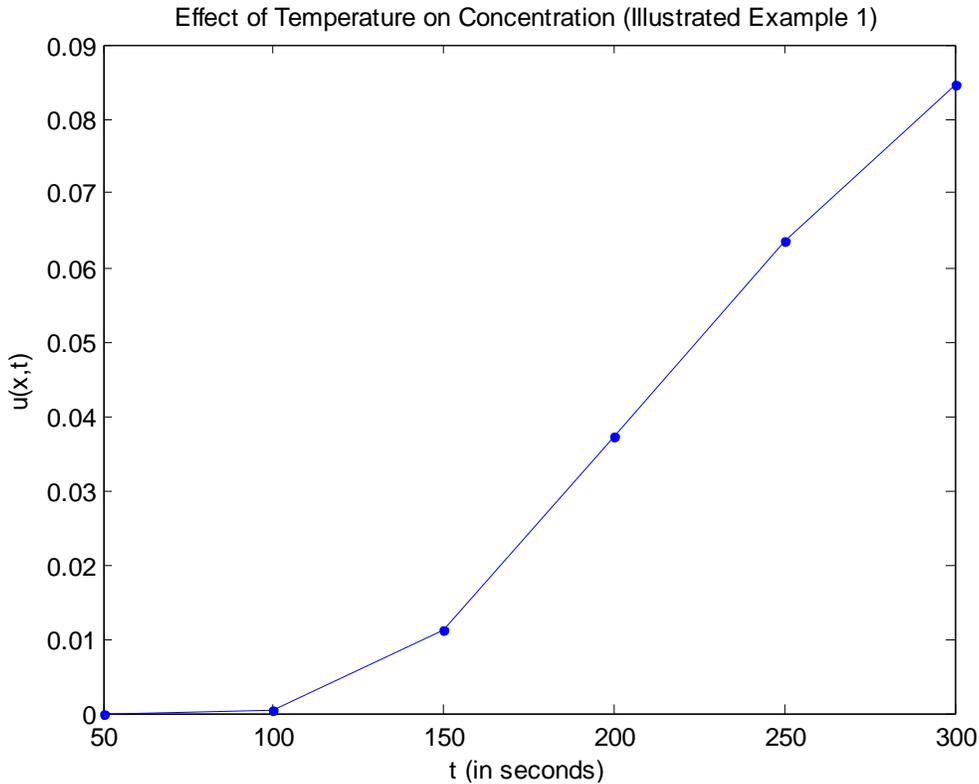


Figure 8: A graph showing the effect of the temperature on concentration from 773k-4773k at given points of x and t.

temperatures (from Table 4) and their corresponding diffusion coefficients. If the surface concentration is maintained at 0.2 wt% Cu. The concentrations from 2mm to 12mm from the surface after 50 seconds to 300 seconds respectively are simulated as shown in Table 6 and shown on plots in Figure 8.

$$\text{From (15): } u(x, t) = (u_s - u_0) \left[1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \right] + u_0 \quad (17)$$

CONCLUSION

This study evaluated the effect of temperature on concentration of a conductive material. From the investigation, the following observations have been drawn.

(1) From the figures 2, 4 and 6, the diffusion coefficients increased as a result of significant increase in the temperatures from 773 to 4773K.

(2) Figure 8 showed that the concentration of the material increased due to diverse increase in temperatures. Most materials that allow operation at high temperature are essential in most industries from material producing and processing to transportation and power generation. There is a need for varying the data parameters by decreasing the temperatures to investigate their effect on the concentration of the modelled conductive material.

(3) High temperature reduces material stiffness and strength while low temperature increases material stiffness and strength.

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