

Transient Analysis of Thermal Treatment Processes Carburizing and Nitriding of Steel Components by Numerical Modeling and Simulation



Swathi Boosala, Srikanth Satish Kumar Darapu, M.Nagendrababu, Ch.Suresh

Abstract: The purpose of carburizing, nitriding and carbonitriding is to increase the strength of components. Elements such as carbon, nitrogen and carbon-nitride are diffused into the components at high temperature convective environment. The amount of diffusion is to be regulated by controlling the temperature and time of diffusion. Time and temperature of process govern diffusion rate and strength of the component. Numerical modeling is applied by energy balance approach i.e., equating rate of change of energy is equal to energy transferred by conduction, convection and radiation. By non dimensionalising relations for the mentioned critical parameters were obtained. The phenomenon of convection, radiation and conduction are taken together for the purpose of numerical modeling. Variation of temperature and depth of diffusion of component for the taken components i.e., sphere and cube was plotted in transient state. For both numerical analysis and simulation the boundary conditions i.e., for carburization the ambient temperature is 950°C with carbon monoxide as the carburizing agent and for nitriding the ambient temperature is 530°C with nitrogen as nitriding agent and the component taken is of steel which is initially at room temperature were taken. Results obtained from numerical modeling and simulation were compared with each other and observed that in both analyses the variation of temperature with time and depth of diffusion is almost linear. Final differential equation obtained in numerical modeling is a single order non linear differential equation which is solved in MATLAB using finite difference approach. Data obtained from MATLAB were plotted for variation of surface temperature and geometric dimension with respect to time.

Keywords: carburization, nitriding, mass diffusion, energy balance, numerical modeling, simulation, critical parameters.

Nomenclature

$\frac{d}{dt}[m c_p(T - T_o)]$ = heat transferred at any instant.

$h_{conv}[T_g - T]A$ = Heat transferred by convection

$\epsilon C_o A [T_g^4 - T^4]$ = Heat transferred by radiation

$m = \frac{4}{3}\pi R^3 \rho$ mass of the component

$A = 4\pi R^2$

Fo: Fourier Number $\frac{\alpha \tau}{R^2}$

$A = 4\pi R^2$: surface area of the component

$$R^* = \frac{r}{R'}$$

$$T^* = \frac{T(t)}{T_o}$$

$$T_o^* = \frac{T_i}{T_o}$$

$$k_1 = \frac{h_c R_i}{k}$$

$$k_2 = \frac{\epsilon C_o R T_o^3}{k}$$

$$k_3 = \frac{d[\rho - \rho_\infty]}{\alpha \rho}$$

d = mass diffusivity coefficient $\frac{m^2}{s}$

ρ = density of material at interface

ρ_∞ = density of gas

$m = s^3 \rho$ mass of the component

$A = 6s^2$

Fo: Fourier Number $\frac{\alpha \tau}{s^2}$

$A = 6s^2$: surface area of the component

$$k_3 = 2 \frac{h_m s [\rho - \rho_\infty]}{\alpha \rho}$$

$$k_1 = \frac{2 h_c R_i}{k}$$

$$k_2 = \frac{2 \epsilon C_o R T_o^3}{k}$$

$$k_3 = \frac{2 d [\rho - \rho_\infty]}{\alpha \rho}$$

$C_1 = k_1/k_3$

$C_2 = k_2/k_3$

$$k_1 = \frac{h_c R_i}{k}, k_2 = \frac{\epsilon C_o R T_o^3}{k}$$

Gr: Grashoff number

Pr: Prandtl number

g : Acceleration due to gravity

t_m = time taken (sec)

t_s = surface temperature ($^{\circ}C$)

r = radius of the sphere component (m)

S = length of side of cube (m)

I. INTRODUCTION

Gas carburizing is used for surface hardening of steel. The quality of carburized parts is determined by hardness of the component and case depth of the diffused element i.e. carbon into the upper layers of the component. Present gas carburizing processes are facing challenges in controlling depth and temperature of the component by carburizing environment. This drawback leads to improper machining and greater tear and wear of the component.

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It is known that the carburizing, nitriding and carbo nitriding are metallurgical surface modification techniques which induce the elements such as carbon and nitrogen into the interstitial spaces between the voids of parent element. These processes results in increasing the surface hardness and modulus (stiffness) of the material. Carbonitriding helps in decreasing the slip of the material during machining processes. This process is applied to less expensive material like low carbon steel. Case hardening treatment is followed for getting this process done [1]. For the purpose of induction of carbon components which are rich in carbon such as charcoal and for that of nitrogen urea are used. As that of carburizing carbonitriding is also carried out by gas carburization process. It is carried out slightly greater than nitriding (530°C) and lesser than plain carburizing (950°C) i.e., at temperature 850°C. The thickness of the layer formed over the surface of the component ranges from 0.07mm to 0.5mm. Depending upon the strength requirement of the material the thickness can be varied. Thickness beyond the range may result in over hardness of the material hence making it brittle.

The thickness of the element diffused need to be regulated which is done by calculating the critical time [2][7]. The necessary formulation for computing this critical time is done by numerical modeling as shown below. As the time of thermal treatment and thickness of the layer are main influencing parameters of the strength of the component hence the variation of each parameter with respect to time were observed and inferences were given[8][9]. Fick's law of diffusion is used for the purpose of solving mass transfer equation in this problem. This law is of the form partial parabolic differential equation. Instead of mass transfer coefficient diffusion coefficient is used and mass balance will applied between the fluxes. [3]. Numerical modeling for mass diffusion into a porous medium will be complex hence the mass diffusion in this problem is constrained to metallic components where voids between the atoms of the parent component are created due to thermal treatment and these are filled by the surrounding gas elements such as carbon or nitrogen. The phase of the material during heat treatment may alter which affect the rate of diffusion hence the phase is considered to be constant so that mass diffusion also remains constant. But porous materials with phase changing capability are having enhanced thermal conductivity and heat transfer by 3-500 times when compared to former ones [6]. Mass transfer plays a vital role in drying of paper. The governing parameters in this case are velocity of the hot air flowing over the surface of the paper and temperature of the convective atmosphere. Since paper is a porous media the rate of mass transfer from surface to surrounding atmosphere will be very high. Skin friction coefficient is also considered in this scenario [7].

For any heat treatment process all the three modes of heat transfer i.e., conduction, convection and radiation will be remains constant.

accounted. But depending upon the temperature encountered in the process any two of these phenomena will be predominant. For example when a metallic component is considered the primary mode of heat transfer is through conduction. If the temperature of the surrounding atmosphere is of higher order then radiation will come into existence. And if the surrounding atmosphere is comprised of some gases and they flowing at some velocities convective heat transfer will also takes part. When these three modes were considered then the thermal resistances offered by these three modes influence the rate of heat transfer.

II. ASSUMPTIONS

- The material of the fin is isotropic in nature.
- Temperature variation is along the surface of the cylindrical fin only.
- Heat transfer is taking place in one dimension only.
- Transient analysis is in one dimension.
- Specific heat of the parent material remains constant throughout the thermal treatment.
- The phase of the material doesn't change during heating of the component.
- Mass diffusion into the material remains constant throughout the process.
- The gas is supplied at constant temperature.
- The component is not allowed to reach its recrystalline temperature.
- Convective atmosphere between the component and gas is of natural convection
- The shape factor of the component with respect to the furnace used for heating is unity
- Emissivity of the material remains constant throughout the process.

III. DESCRIPTION

The components considered for modeling simple geometries sphere and cube. For thermal treatment processes any type of geometry can be considered as they can be applied for wide range of components [5]. But the components will undergo dimensional deformation due to heating. The gases considered for carburization and nitriding are carbon monoxide and nitrogen. The respective thermal properties for the gases were taken from heat transfer data book by Kodandaramam. Material used for analysis is steel. The properties of materials used in analysis were tabulated below [6]. The heat transfer coefficient for both the heat treatment processes carburizing and nitriding is assumed to be constant. Because there is temperature variation in the surface of the component but the temperature of the ambient gas remains constant hence the thermal properties of the gas also

Table 1: properties of material and gases used in carburization and nitriding

Thermal property name	Carbon monoxide	nitrogen	Steel
Chemical formula	CO	N ₂	-
Temperature of ambience(°C)	950	530	-
Thermal diffusivity(m ² /s)	230*10 ⁻⁶	120.834*10 ⁻⁶	1.172*10 ⁻⁵

Thermal conductivity (W/m ² -K)	0.08	0.057	43
Prandtl number	0.742	0.677	-
Density of the element (kg/m ³)	0.28	0.43	7700
Kinematic Viscosity of the gas(m ² /s)	169*10 ⁻⁶	82.12*10 ⁻⁶	-
Specific heat (J/kg-K)	1040	1040	420

There are no external power source for convection hence it is assumed to be free convection. Convective heat transfer coefficient is evaluated by taking the below correlation.

$$Nu = 2 + 0.43(Gr \cdot Pr)^{0.25}$$

$$Gr = \frac{g\beta\Delta t l^3}{\nu^2}$$

IV. NUMERICAL MODELLING

Energy balance for the given process is as follows. The influence of convection and radiation are predominant due to strong convective currents. The diffusion of carbon and nitrogen varies radially from outer surface to some depth. Hence the radius of the component is also assumed to be a varying parameter [3].

On applying energy balance for sphere component following equations are obtained.

$$\frac{d}{d\tau}[mc_p(T - T_o)] = h_{conv}[T_g - T]A + \varepsilon c_o A [T_g^4 - T^4]$$

The respective formulae for mass and area are substituted in the given energy balance equation.

$$\frac{d}{d\tau} \left[\frac{4}{3} \pi r^3 \rho c_p (T - T_i) \right] = h_{conv} [T_\infty - T] * 4\pi r^2 + \varepsilon c_o * 4\pi r^2 * [T_\infty^4 - T^4] \quad (1)$$

After attaining the energy balance the respective parameters are non dimensionalised for the purpose of easy integration. By applying non dimensional formulae the above equation reduces to

$$\frac{d}{dFo} [R^3(T^* - T_o^*)] = \frac{3h_c R}{\alpha \rho c_p} R^{*2} (1 - T^*) + \frac{3\varepsilon c_o R T_\infty^3}{\alpha \rho c_p} R^{*2} (1 - T^{*4}) \quad (1)$$

Where k1 and k2 are assumed to be constant.

After Substituting the equation reduces to as follows:

$$\frac{dT^*}{dFo} = \frac{3k_1}{R^*} (1 - T^*) + \frac{3k_2}{R^*} (1 - T^{*4}) + \frac{dR^*}{dFo} * \frac{3}{R^*} (T^* - T_o^*) \quad (2)$$

Applying Boundary Conditions:

$$Fo = 0, T^* = T_o^*, R^* = 1$$

Now considering mass transfer:

Mass of element diffused at any instant = mass of the element diffused at interface + mass of the surrounding.

$$\frac{d}{d\tau} \left[\frac{4}{3} \pi r^2 \rho \right] = \frac{d[\rho - \rho_\infty]}{R} * 4\pi r^2 \quad (3)$$

$$\frac{dR^*}{dFo} = k_3$$

Therefore, the governing equations are:

$$\frac{dT^*}{dR^*} = \frac{\frac{3k_1}{R^*}(1-T^*) + \frac{3k_2}{R^*}(1-T^{*4}) + \frac{3k_3}{R^*}(T^* - T_o^*)}{k_3} \quad (6)$$

$$\frac{dR^*}{dFo} = k_3 \quad (7)$$

$$\frac{dT^*}{dFo} = \frac{3k_1}{R^*} (1 - T^*) + \frac{3k_2}{R^*} (1 - T^{*4}) + \frac{3k_3}{R^*} (T^* - T_o^*) \quad (8)$$

On applying energy balance for cubical component following equations are obtained.

$$\frac{d}{d\tau} [mc_p(T - T_o)] = h_{conv}[T_g - T]A + \varepsilon c_o A [T_g^4 - T^4] \quad (9)$$

The respective formulae for mass ad area are substituted in the given energy balance equation.

$$\frac{d}{d\tau} [x^3 \rho c_p (T - T_i)] = h_{conv} [T_\infty - T] * 6x^2 + \varepsilon c_o * 6x^2 * [T_\infty^4 - T^4] \quad (10)$$

After attaining the energy balance the respective parameters are non dimensionalised for the purpose of easy integration.

$$s^* = \frac{x}{s}, T^* = \frac{T(t)}{T_\infty}, T_o^* = \frac{T_i}{T_\infty} \quad (11)$$

By applying non dimensional formulae the above equation reduces to

$$\frac{d}{dFo} [s^{*3}(T^* - T_o^*)] = \frac{6h_c s}{k} s^{*2} (1 - T^*) + \frac{6\varepsilon c_o s T_\infty^3}{k} s^{*2} (1 - T^{*4}) \quad (12)$$

$$\frac{dT^*}{dFo} = \frac{k_1}{s^*} (1 - T^*) + \frac{k_2}{s^*} (1 - T^{*4}) + \frac{dR^*}{dFo} * \frac{1}{s^*} (T^* - T_o^*) \quad (13)$$

Applying Boundary Conditions:

$$Fo = 0, T^* = T_o^*, s^* = 1$$

Now considering mass transfer:

Mass of element diffused at any instant = mass of the element diffused at interface + mass of the surrounding.

$$\frac{d}{d\tau} [x^3 \rho] = \frac{d[\rho - \rho_\infty]}{s} * 6x^2 \quad (14)$$

$$\frac{ds^*}{dFo} = k_3$$

Therefore, the governing equations are:

$$\frac{dT^*}{ds^*} = \frac{\frac{3k_1}{s^*}(1-T^*) + \frac{3k_2}{s^*}(1-T^{*4}) + \frac{3k_3}{s^*}(T^* - T_o^*)}{k_3} \quad (17)$$

$$\frac{ds^*}{dFo} = k_3 \quad (18)$$

$$\frac{dT^*}{dFo} = \frac{3k_1}{s^*} (1 - T^*) + \frac{3k_2}{s^*} (1 - T^{*4}) + \frac{3k_3}{s^*} (T^* - T_o^*) \quad (19)$$

If the phenomenon of conduction is also considered then numerical modeling will be as follows.

$$\begin{aligned} \frac{d}{d\tau} [mc_p(T - T_o)] &= h_{conv}[T_g - T]A + \varepsilon c_o A [T_g^4 - T^4] + \\ kA \frac{dT}{dr} & \\ \frac{d}{d\tau} [x^3 \rho c_p (T - T_i)] &= h_{conv} [T_\infty - T] * 6x^2 + \varepsilon c_o * 6x^2 * [T_\infty^4 - T^4] + k6x^2 \frac{dT}{dr} \end{aligned}$$

On non - dimensionalising and regrouping final equations are as follows:

$$\frac{dT^*}{dR^*} = \frac{c1(1-T^*) + c2(1-T^{*4}) + (T^* - T_o^*)}{(\frac{R^*}{3} + \frac{1}{k_3})}$$

$$\frac{dR^*}{dFo} = k_3$$

Similarly for cube

$$\frac{dT^*}{dR^*} = \frac{c1(1 - T^*) + c2(1 - T^{*4}) + (T^* - T_o^*)}{\left(\frac{s^*}{3} + \frac{2}{k3}\right)}$$

$$\frac{dR^*}{dFo} = k_3$$

Complete numerical modeling of component of any dimension and any geometry is simplified such that if its volume is able to computed. Any complex geometry can be modeled numerically if control volume is written. It is observed that the variation of depth of diffusion of carburization or nitriding with time is deduced to a constant which is dependent on properties of gas that is being used. [4]

V. RESULTS AND DISCUSSIONS

The above non linear first order differential equations are solved in MATLAB and the following graphs were plotted. Graphs for temperature, radius and time for carburization and nitriding for the both spherical and cubical components were plotted with and without conduction. Plots for the above parameters are mostly exponential. Graphs for time and surface temperature of the components in carburization and nitriding without conduction follow exponential trend line whereas when conduction is considered they show almost linear fashion. The maximum time for formation of 1mm to 5mm thick layer of carburization or nitriding is about 15 to 20 min. Simulation for temperature variation with temperature was done in ANSYS in transient state for 1000 iterations. The corresponding diagrams in carburization and nitriding were shown. If the time of the thermal treatment process is controlled hence the strength of the component can be increased effectively without changing the initial mechanical properties of the material. When conduction is not considered the maximum temperature of the process is reached within 50 min. Hence the time taken for the material to reach its recrystalline temperature is noted and is seen that the material exposed to the treatment below that temperature. For the purpose of overcoming this problem all thermal treatment processes were done for maximum of 1000 seconds.

All bodies above 0⁰K emit radiation. It is a known fact. But as the temperature goes on increasing the influence of conduction will be reduced. Hence in this paper the analysis was carried out with and without conduction so that the role of conduction at higher temperatures can be easily predicted. Since the components taken for thermal treatment process are metallic solids and the prime mode of heat transfer in solids in thorough conduction even at higher temperature it played vital role temperature variation and mass diffusion. The mechanism of heat transfer for surrounding gas to the component is by convection and radiation and within the component only conduction participates for temperature progress. Hence only upper surface of the component will be exposed to maximum temperature as shown in the figure. For attaining same temperature without conduction in carburizing and nitriding time taken for former one less when compared to later. Even for radius of the material reached in carburization is less when compared to nitriding for same time. The slope of the curves for cube when compared to sphere is observed to be more.

3.1 Carburization without conduction

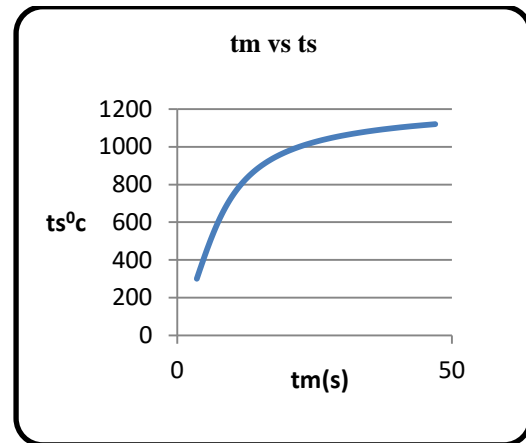


Figure 1 variation of surface temperature with time in carburization without conduction for sphere

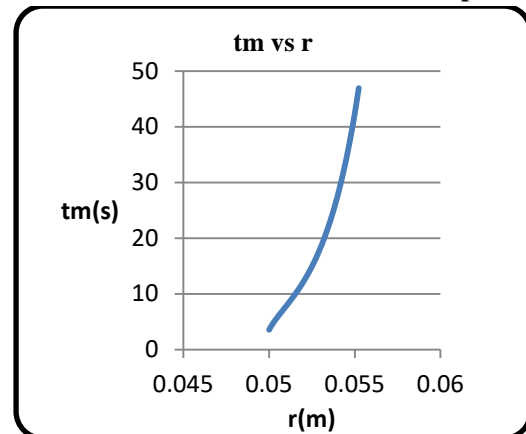


Figure 2 variation of surface temperature with radius in carburization without conduction for sphere

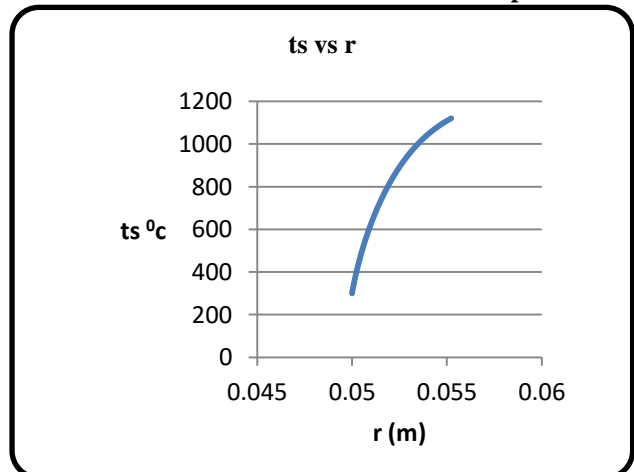


Figure 3 variation of radius with temperature in carburization without conduction for sphere

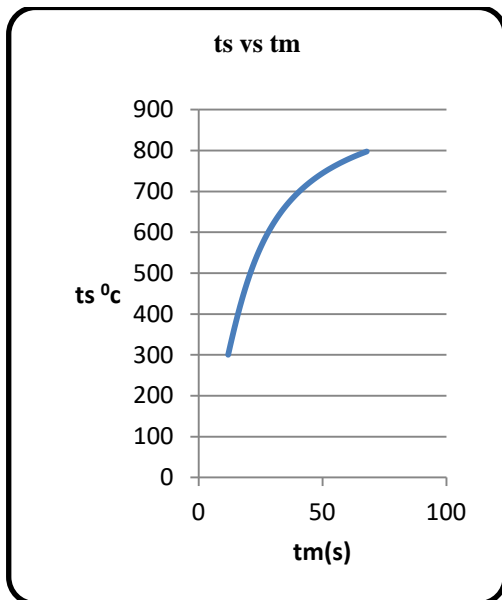


Figure 4 variation of surface temperature with time in nitriding without conduction for sphere

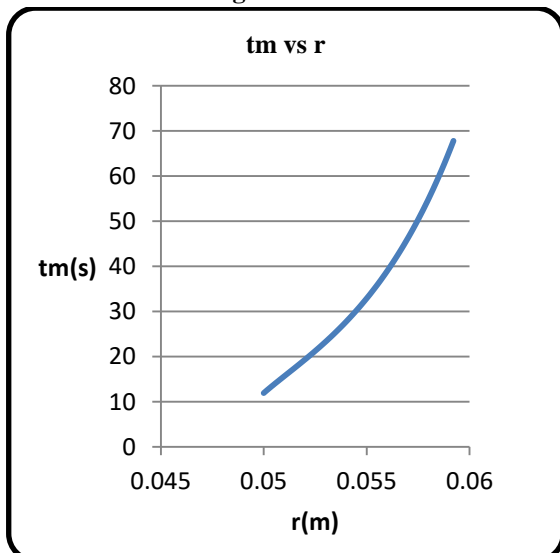


Figure 5 variation of radius with time in nitriding without conduction for sphere

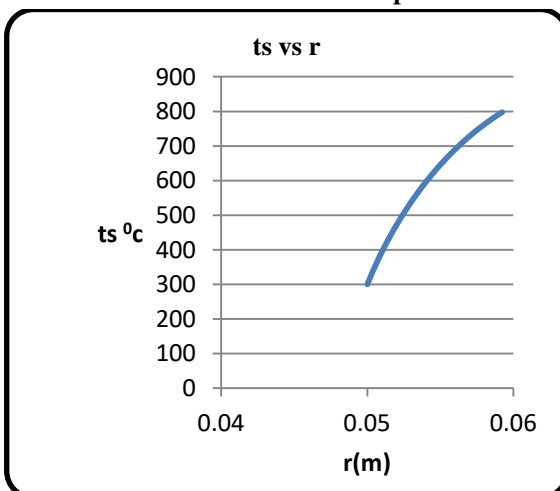


Figure 6 variation of radius with surface temperature in nitriding without conduction for sphere

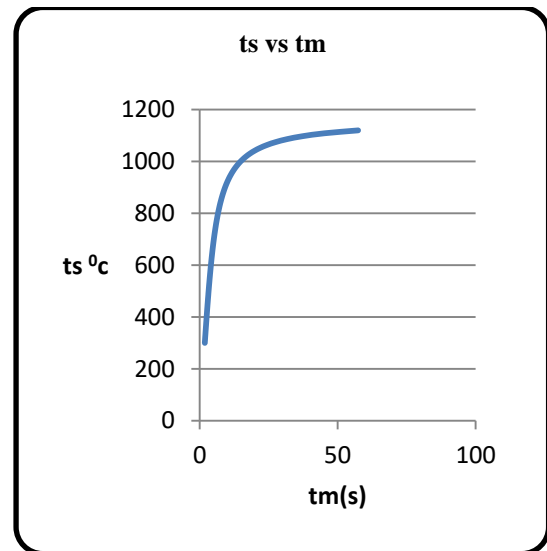


Figure 7 variation of time with surface temperature in carburization without conduction for cube

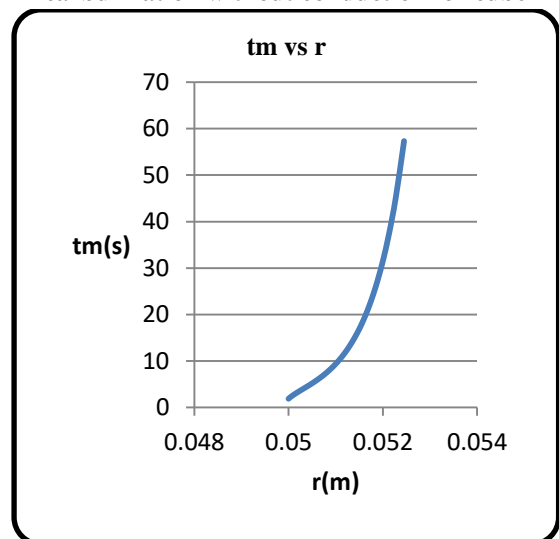


Figure 8 variation of time with radius in carburization without conduction for cube

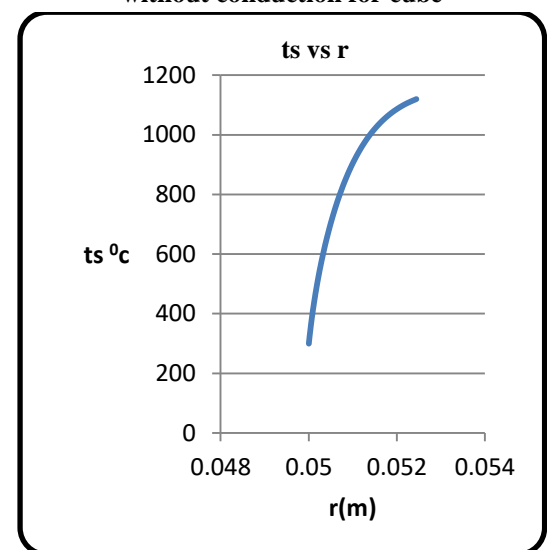


Figure 9 variation of side with surface temperature in carburization without conduction for cube

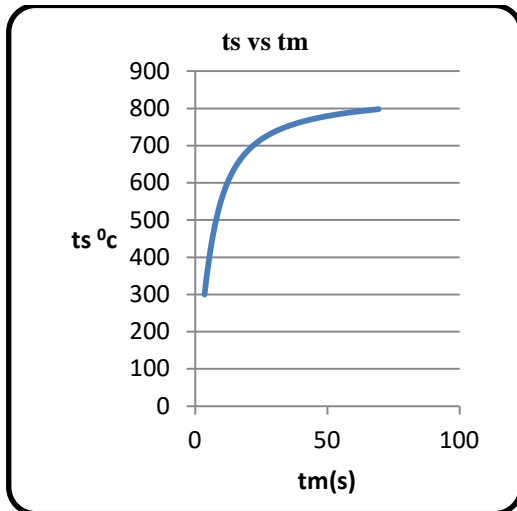


Figure 10 variation of time with surface temperature in nitriding without conduction for cube

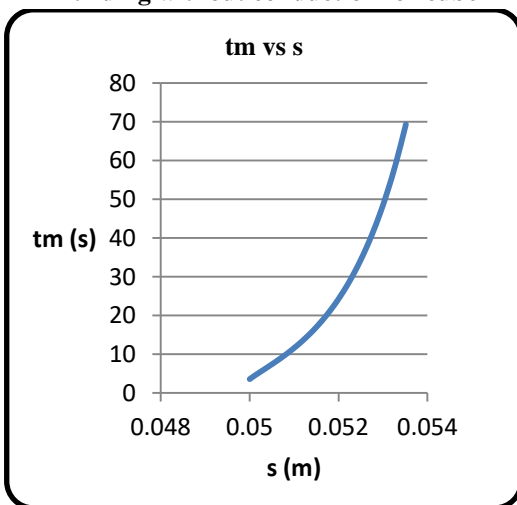


Figure 11 variation of time with temperature in nitriding without conduction for cube

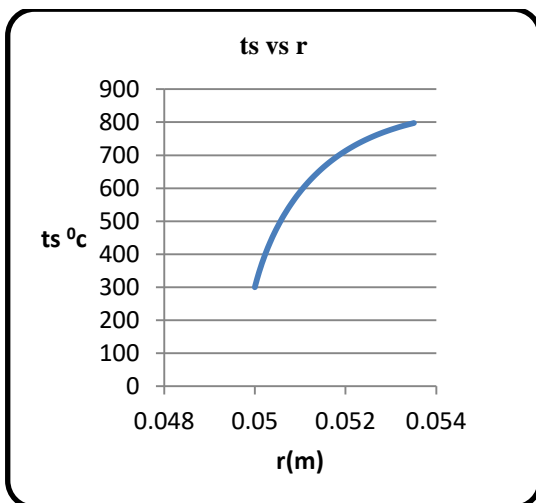


Figure 12 variation of side with surface temperature in nitriding without conduction for cube

3.3 Carburization with conduction

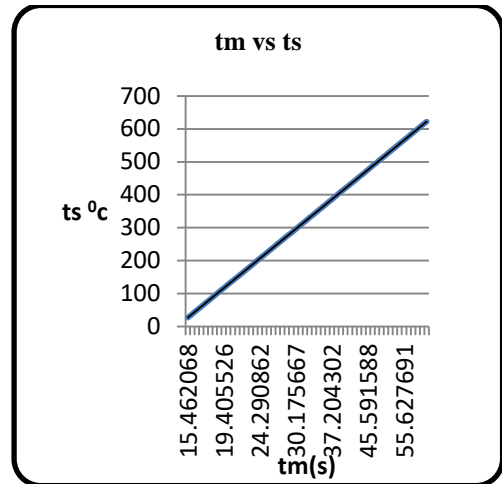


Figure 13 variation of time with surface temperature in carburization with conduction for sphere

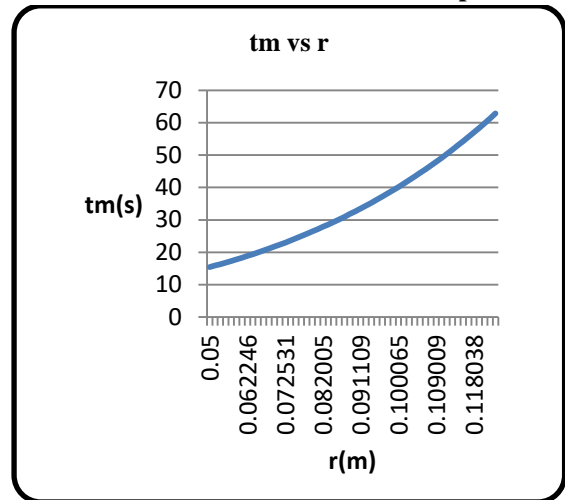


Figure 14 variation of time with radius in carburization with conduction for sphere

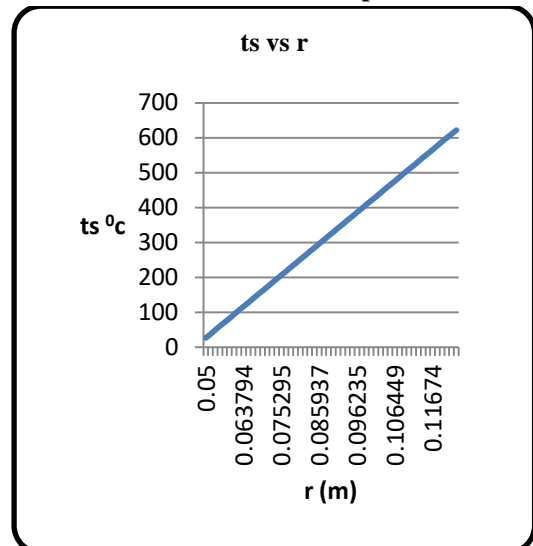


Figure 15 variation of radius with surface temperature in carburization with conduction for sphere

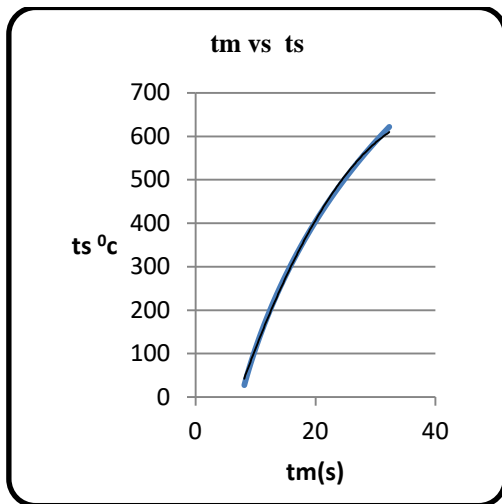


Figure 16 variation of time with surface temperature in carburization with conduction for cube

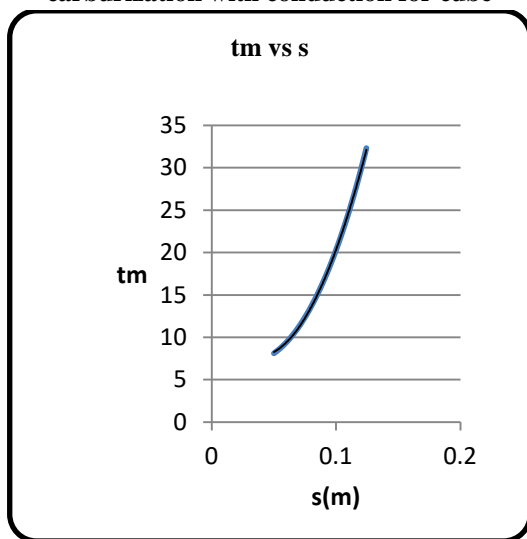


Figure 17 variation of time with side in carburization with conduction for cube

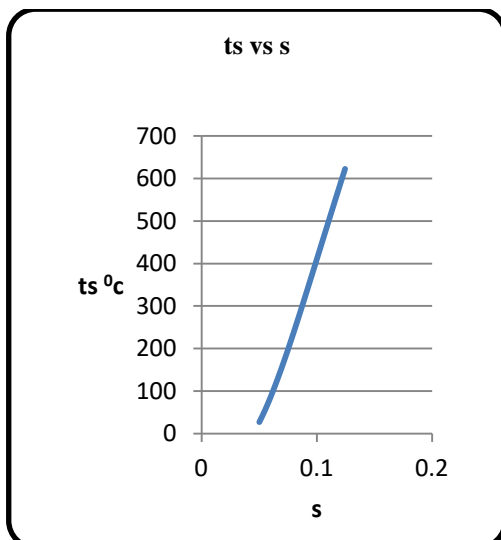


Figure 18 variation of side with surface temperature in carburization with conduction for cube

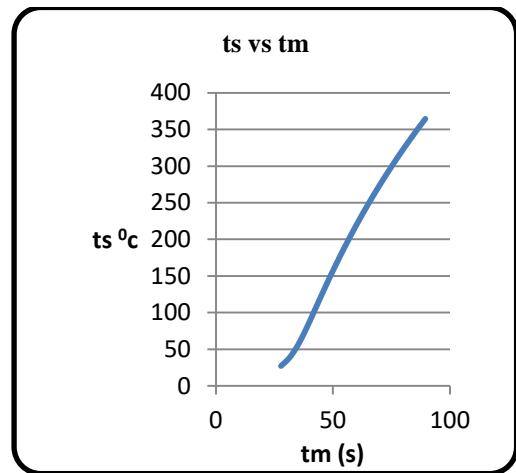


Figure 19 variation of time with surface temperature in nitriding with conduction for cube

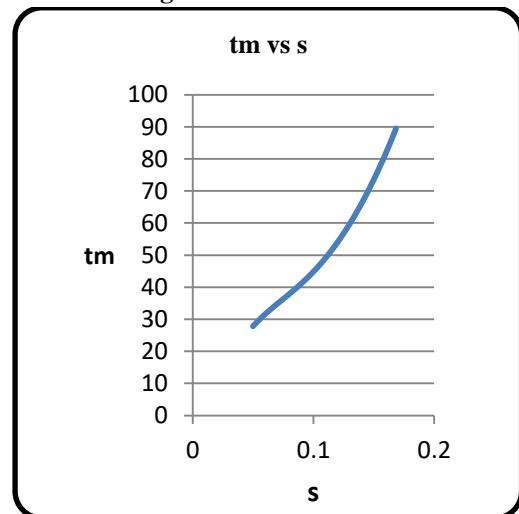


Figure 20 variation of time with side in nitriding with conduction for cube

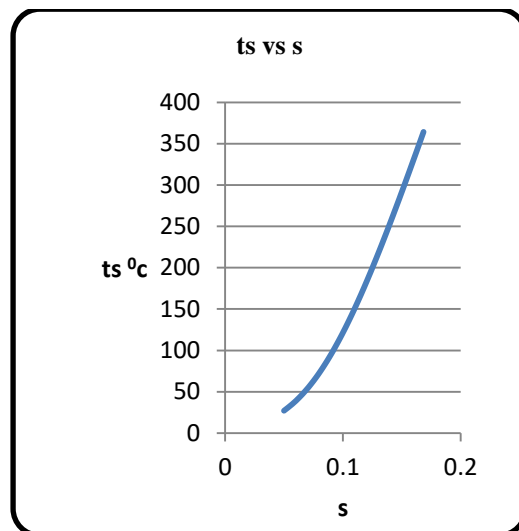


Figure 22 variation of side with surface temperature in nitriding with conduction for cube

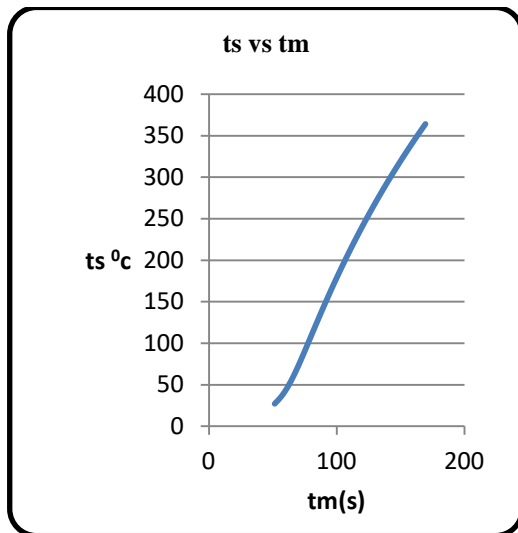


Figure 23 variation of time with surface temperature in nitriding with conduction for sphere.

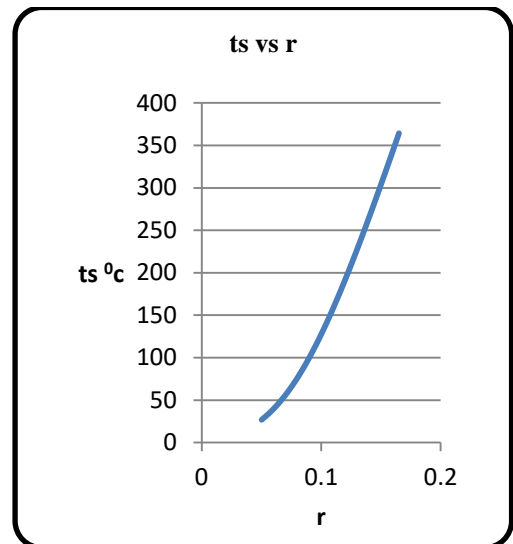


Figure 25 variation of time with radius in nitriding with conduction for sphere

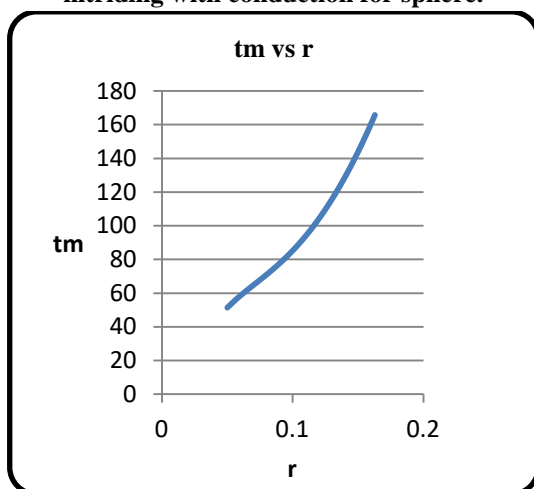


Figure 21 variation of radius with time in nitriding with conduction for sphere.

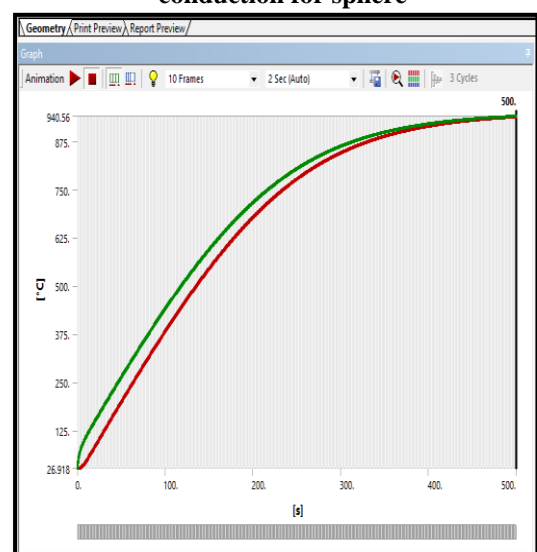


Figure 26 variation of temperature for cube with conduction in carburization carried out for 500sec in ANSYS

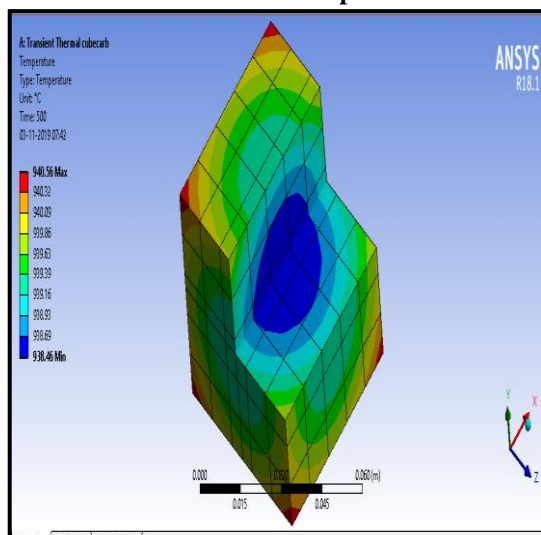


Figure 24 sectional view of cube with conduction in carburization carried out for 500sec in ANSYS

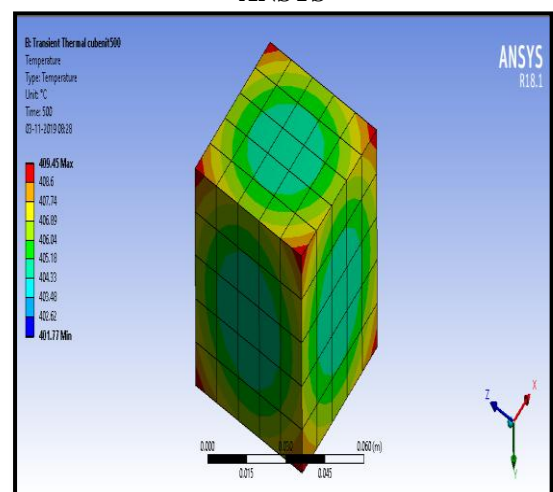


Figure 27 cube with conduction in nitriding carried out for 500sec in ANSYS

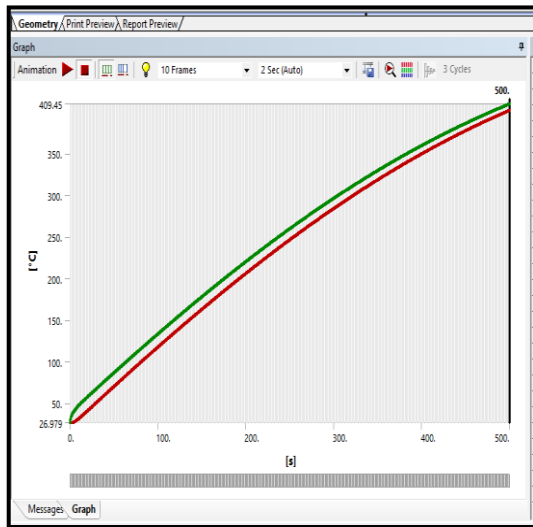


Figure 28 variation of temperature for cube with conduction in nitriding carried out for 500sec in ANSYS

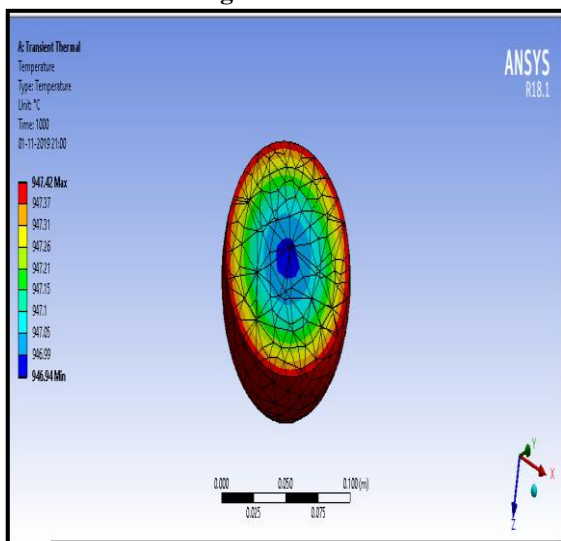


Figure 29 sectional view of sphere with conduction in carburization carried out for 1000 sec in ANSYS

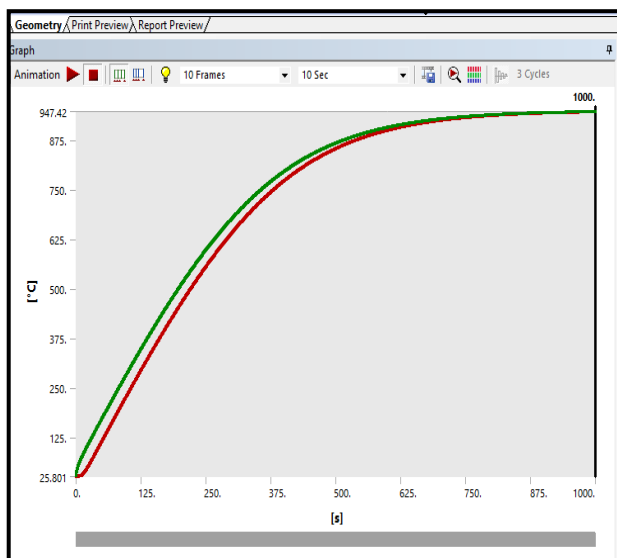


Figure 30 variation of temperature for sphere with conduction in carburization carried out for 1000 sec in

ANSYS

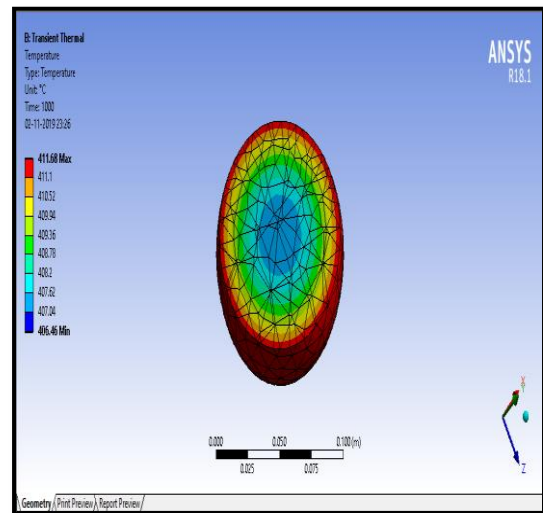


Figure 31 sectional view of sphere with nitriding in carburization carried out for 1000 sec in ANSYS

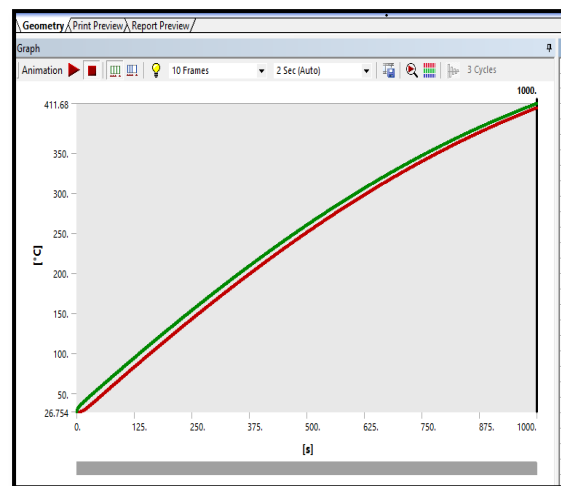


Figure 32 Variation of temperature for sphere in carburization for 1000 sec

Graphs for variation of temperature both in simulation and numerical modeling for the chosen components sphere and cube of steel in carburization and nitriding show same behavior. They almost vary linearly with time in both cases. Hence simulation results and numerical modeling results are efficiently comparable. They show little deviation. Due to less temperature of ambience in nitriding process the variation of temperature is almost linear when compared to that of carburization process. The time to reach the ambient temperature is very less when compared to former one. In case of carbo nitriding initial for first 5 to 7 minutes plain gas carburization will be carried out and for the last 5 minutes only nitriding will be carried out. The temperature of the component for thickness of 0.07 mm to 1mm is observed to be 350°C to 400°C in carburization and for that of nitriding it is 200°C to 250°C

Table 2: Maximum values of temperature and depth of diffusion obtained for specified time

Name of the process	Time (sec)	Temperature (°C)	Dimension (m)
Carburization without conduction for sphere	50	827	0.055
Nitriding without conduction for sphere	70	527	0.06
Carburization without conduction for cube	50	827	0.052
Nitriding without conduction for cube	75	527	0.054
Carburization with conduction for sphere	52	600	0.058
Nitriding with conduction for sphere	60	350	0.057
Carburization with conduction for cube	30	600	.06
Nitriding with conduction for cube	35	350	0.06

Above table gives comparison values of maximum surface temperature attained and depth of diffusion of carbon and nitrogen into the spherical or cubical component within the given time of thermal treatment.

VI. CONCLUSIONS

- Variation of temperature with time for both nitriding and carburizing is linear.
- Any complex geometry can be modelled if their volume is known.
- Depending upon the application control over thickness of the deposited carburized and nitride layer can be attained.
- Time taken for specified temperature and radius can be easily computed.
- Above numerical analysis can be employed for any thermal treatment processes such as carbo nitriding and decarburizing.
- Results attained thorough this numerical modelling are satisfactory with those of standard values in carburization and nitriding.
- Over heating of the component can be easily regulated hence attaining of recrystalline temperature of the component material is almost prevented due to regulation over time of treatment.
- Brittleness of the material is reduced due to regulation over thermal diffusion of the element.
- Depth of diffusion of carbon or nitrogen can be easily known depending upon the strength of the component.

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