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To cite this article: A H Norzilah and N Rusli 2020 *IOP Conf. Ser.: Mater. Sci. Eng.* **767** 012021

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Prediction of carbon concentration profile within carburised-carbon steel 1024 using Alternating Direction Implicit (ADI) method

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Abstract. Pack carburisation is recognised to improve the carbon surface content of carburised-carbon steel 1024 that enhance the surface hardness and further can be used in automobiles, form implements, machines, gears and springs. The transient two-dimensional diffusion equation that represents the carbon concentration profile within the carburised-carbon steel 1024 is discretised using Alternating Direction Implicit (ADI) technique. A semi-analytical method is used to verify the ADI method and the numerical algorithm is developed in MATLAB software. To materialise the pack carburisation process, the boundary condition, initial condition and step time are encoded to signify the experiment conditions from the literature. The simulation results successfully predicted the carbon concentration profile within the carburised-carbon steel 1024 with variation of carburisation time (2 hours to 60 hours) and temperature (900°C - 1000°C). The effect of carburisation time and temperature are evaluated and the relation of both effects on the carbon development is explained. Simulation results show that carburisation extended to 60 hours only increases the carbon content at the core to 0.3wt% from 0.24 wt% of its original content. The small increment is satisfactory to maintain its ductility by hardening the surface.

1. Introduction

Pack carburisation is categorised as a heat treatment for surface hardening of low carbon steel 1024. According to American Iron and Steel Institute/Society of Automotive Engineers (AISI/SAE) steel grade, -10 represents the categorisation of plain carbon steel and 24-denotes the weight percentage of carbon content which is 0.24wt%. Because of its low carbon content, surface hardening is necessary to increase the carbon content hence to be used in applications such as arbours, hinges, link components, driving pins, camshafts and cardan joints. These applications require only the surface to be hardened by maintaining the core ductility.

The carbon steel is packed with a mixture of solid carburiser, such as charcoal, activated carbon or graphite powder, along with energiser in the carburisation box. Then the prepared box is exposed at high temperature ranges from 900 to 1000°C for 2 to 12 hours. The process involves 4 stages - the oxidation between the air with the packed carbon, the decomposition of carbon monoxide gas, the deposition of carbon on the steel surface and finally the carbon diffusion within the steel structure at high temperature.



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Improvement of surface hardness of low carbon steel is theoretically instigated by the rapid cooling of carburised layer resulted from the carburisation. Nevertheless, often found in the literature the surface hardness reading is presented without demonstration of carbon concentration profile at corresponding depths [1-3]. In practice, carbon content at each depth is measured using spark emission spectroscopy once pack carburisation process completed. However, the measurement is restricted to a certain depth. On top of that, it is difficult and time-consuming to control the desired carbon concentration on the surface of low carbon steel experimentally.

It is established that the carburisation process is dominated by diffusion. Thus, understanding about the carbon diffusion during carburisation is crucial in order to determine the effective case depth and this is the reason why the carbon profile concentration is essential. The carbon concentration profile is resulted from the carbon diffusion equation recognised as Fick's Second Law. The Fick's Second Law is a parabolic partial differential equation that represents the relationship between the rate of carbon concentration with the diffusivity and the carbon concentration gradient.

One of the techniques from finite difference method to solve the two-dimensional transient or unsteady-state of Fick's Second Law is Alternating Direction Implicit (ADI). The technique is basically initiates with breaking the 2-D problems into the 1-D problem and solves each problem implicitly. It is unconditionally stable and also overcomes the drawbacks of the normal implicit finite difference method which is very time-consuming and less efficient. The technique has proven to be more efficient and stable in solving parabolic and elliptic differential equation compared to the implicit scheme alone [4,5]. The heat or mass equation is closely represented the physical or chemical processes occurred in engineering. Determination of dependent variables such as temperature and concentration within the solid or fluid in multi-dimension are essential in order to analyse the process in details prior to design purposes.

For example, detailed studies of heat and mass transfer during the drying process of a square cylinder for confined flow are visualised by the usage of ADI-based software [6]. The 2-dimensional numerical analysis is reported comparable with the experimental data. A more complicated process from coupling the heat equation with the continuity equation and carbon dioxide (CO₂) properties during tubing and annulus injection also solved by ADI method. As a result, Zhao et al., successfully estimated the wellbore temperature and pressure profile at the axial and radius direction [7]. Aslib et al., used the ADI method to resolve the transient heat transfer problem of an anisotropic cylindrical pin fin with heat sink. The numerical results stated as well-validated with the analytical solution [8]. The ADI method also exhibited good agreement with the experimental data in more complex heat transfer problem involving Vapour Phase Soldering (VPS) for electronic components [5]. The findings also highlight the potential of the ADI method in advanced manufacturing engineering application.

Therefore, this paper presents the application of ADI method in solving transient 2-dimensional diffusion equation to visualise the carbon concentration growth within the carbon steel 1024 during pack carburisation. The discretised algorithm is validated with semi-analytical method and then used to evaluate the carbon concentration at various carburisation temperature and time.

2. Methodology

2.1 Discretisation of transient two-dimensional diffusion equation

The transient two-dimensional diffusion equation is given by equation (1):

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) \quad (1)$$

Using ADI formulation, Equation (1) is discretised to:

$$\frac{C_{i,j}^{n+\frac{1}{2}} - C_{i,j}^n}{\left(\frac{\Delta t}{2}\right)} = D \left[\frac{C_{i+1,j}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i-1,j}^{n+\frac{1}{2}}}{(\Delta x)^2} + \frac{C_{i,j+1}^n - 2C_{i,j}^n + C_{i,j-1}^n}{(\Delta y)^2} \right] \quad (2)$$

and

$$\frac{C_{i,j}^n - C_{i,j}^{n+\frac{1}{2}}}{\left(\frac{\Delta t}{2}\right)} = D \left[\frac{C_{i+1,j}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i-1,j}^{n+\frac{1}{2}}}{(\Delta x)^2} + \frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{(\Delta y)^2} \right] \quad (3)$$

Where Δt = time step size; Δx = x step size; Δy = y step size; n = time level; i and j = Cartesian coordinates x and y .

Equation (2) and (3) are written in the tridiagonal form as:

$$-d_1 C_{i-1,j}^{n+\frac{1}{2}} + (1+2d_1) C_{i,j}^{n+\frac{1}{2}} - d_1 C_{i+1,j}^{n+\frac{1}{2}} = d_2 C_{i,j+1}^n + (1-2d_2) C_{i,j}^n + d_2 C_{i,j-1}^n \quad (4)$$

and

$$-d_2 C_{i,j-1}^{n+1} + (1+2d_2) C_{i,j}^{n+1} - d_2 C_{i,j+1}^{n+1} = d_1 C_{i+1,j}^{n+\frac{1}{2}} + (1-2d_1) C_{i,j}^{n+\frac{1}{2}} + d_1 C_{i-1,j}^{n+\frac{1}{2}} \quad (5)$$

$$\text{where } d_1 = \frac{1}{2} d_x = \frac{1}{2} \frac{D\Delta t}{(\Delta x)^2} \text{ and } d_2 = \frac{1}{2} d_y = \frac{1}{2} \frac{D\Delta t}{(\Delta y)^2}$$

The solution procedure starts with the solution of tridiagonal system in equation (4). The formulation of this equation is implicit in the x -direction and explicit in the y -direction. Thus, the solution at this stage is referred as the x -sweep. Solving the tridiagonal system of equation (4) provides necessary data for the right-hand side of equation (5) to solve the tridiagonal system of equation (5). In this equation, the finite difference equation is implicit in the y -direction and explicit in the x -direction and referred as y -sweep. Numerical algorithm is then developed based on equation (4) and (5).

2.2 Development of numerical algorithm and implementation in MATLAB

Numerical algorithm of ADI are established in matrix form [9]. For x -sweep:

$$\begin{pmatrix} b_1 & c_1 & 0 \\ a_1 & b_1 & c_1 \\ a_1 & b_1 & c_1 \\ 0 & a_1 & b_1 \end{pmatrix} \begin{pmatrix} C_{2,2} \\ C_{3,2} \\ C_{IN-1,2} \end{pmatrix} = \begin{pmatrix} D_1 - a_1 C_{1,2}^{n+\frac{1}{2}} \\ D_1 \\ D_1 \\ D_1 - c_1 C_{IN,2}^{n+\frac{1}{2}} \end{pmatrix} \quad (6)$$

For y -sweep:

$$\begin{pmatrix} b_2 & c_2 & 0 \\ c_2 & b_2 & a_2 \\ c_2 & b_2 & a_2 \\ 0 & c_2 & b_2 \end{pmatrix} \begin{pmatrix} C_{2,2} \\ C_{2,3} \\ C_{2,4} \end{pmatrix} = \begin{pmatrix} D_{2,j=2} - c_2 C_{2,1}^{n+1} \\ D_{2,j=2} \\ D_{2,j=3} \\ D_{2,j=IN-1} - a_2 C_{2,IN}^{n+1} \end{pmatrix} \quad (7)$$

Where

$$a_1 = -d_1; b_1 = (1 + 2d_1); c_1 = -d_1; a_2 = -d_2; b_2 = (1 + 2d_2); c_2 = -d_2;$$

$$D_1 = d_2 C_{i,j+1}^n + (1 - 2d_2) C_{i,j}^n + d_2 C_{i,j-1}^n; D_2 = d_1 C_{i+1,j}^{n+\frac{1}{2}} + (1 - 2d_1) C_{i,j}^{n+\frac{1}{2}} + d_1 C_{i-1,j}^{n+\frac{1}{2}}; IN = \text{Number of } i, \text{ and } JN = \text{Number of } j.$$

The generated solution will be verified the solution from semi-analytical method.

2.3 Verification with the semi-analytical method

Due to the mathematical similarity between the heat conduction and diffusion equation, the numerical algorithm is verified by semi-analytical method for two dimensional heat conduction equation [10]. Therefore, the variable is written as T which is the temperature to be calculated for the square domain of $0 \leq x \leq 3.0$ m, $0 \leq y \leq 3.0$ m, with $k_x = k_y = 1.25$ Btu/(hr.m.°F), $\Delta x = \Delta y = 0.3$ m, at $t = 1.2$ hr. The equation is subjected to the following boundary and initial conditions:

$$T(0, y, t) = T(x, y, t) = T(L_x, y, t) = T(x, L_y, t) = 0 \quad (8)$$

$$T(x, y, 0) = 30 \quad (9)$$

Where L_x and L_y are the lengths of the solution domain in the x and y directions, respectively. The semi-analytical solution for this problem is:

$$T(x, y, t) = \sum_{n=1}^{\infty} \sum_{j=1}^{\infty} A_n \sin \frac{n\pi x}{L_x} \sin \frac{j\pi y}{L_y} \exp \left[- \left(\frac{k_x n^2 \pi^2}{L_x^2} + \frac{k_y j^2 \pi^2}{L_y^2} \right) t \right] \quad (10)$$

$$\text{Where } A_n = \frac{4(30)}{nj\pi^2} \left[(-1)^n - 1 \right] \left[(-1)^j - 1 \right]$$

The verified numerical method is then used to predict the carbon concentration profile.

2.4 Prediction of carbon concentration profile during pack carburisation

2.4.1 Process description of pack carburisation This numerical studies is based on experimental work conducted by Ali et al. which provide detail information of the carburising condition and the carbon steel dimension [1]. Carbon steel 1024 with carbon content of 0.24wt% is pack carburised with charcoal using barium carbonate (BaCO_3) as carburiser. The stainless steel container is filled with the mixture of charcoal powder and BaCO_3 surrounding the carbon steel as illustrated in figure 1. The stainless steel container (2) contained with the charcoal, BaCO_3 (3) and the carbon steel (4) is pack carburised in the muffle furnace (1) that already being heated before that to reach carburisation temperature of 900-950 °C. The dimension of carbon steel is 0.0508m × 0.0127m. The carburisation occurred for 2, 3, 5 and 9 hours before taken out from the furnace and quenched at room temperature. Heat from the muffle furnace is transferred to the carbon atoms from the surface of carbon steel 1024 to its case.

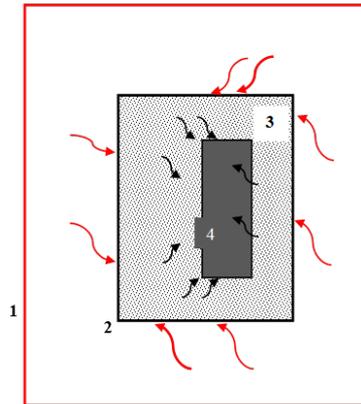


Figure 1. Schematic diagram of pack carburising process in this study

1- Muffle furnace; 2- Stainless steel container; 3 - Mixture of charcoal and barium carbonate; 4 - Carbon steel plate; \rightarrow : Heat conducted from 1 to 2; \blacktriangleright Carbon diffused from 3 to 4.

2.4.2 Mathematical model of pack carburisation The pack carburisation process for carbon diffusion is represented by equation (1). The diffusion coefficient of carbon, D to diffuse into the γ -Fe phase is calculated by equation (11) [11].

$$D(T) = 0.0052 \exp\left(-\frac{127950}{R_j T}\right) \quad (11)$$

Where R_j = Gas constant in 8.314 J/mol.K and T = Temperature in Kelvin (K).

2.4.3 Initial and boundary conditions The initial condition is written as:

$$C_o(x, y, 0) = 0.24 \quad (12)$$

C_o is the initial carbon composition before carburised. The boundary condition for each side of the carbon steel, C_b is written as:

$$C_b(0:0.0508, 0, t) = 1 \quad (13)$$

$$C_b(0:0.0508, 0.0127, t) = 1 \quad (14)$$

$$C_b(0, 0:0.0127, t) = 1 \quad (15)$$

$$C_b(0.0508, 0:0.0127, t) = 1 \quad (16)$$

2.4.4 Computational procedure A computer code is developed in MATLAB. The spatial step size for x and y is 0.0001m respectively and the time step used is 10s. The time step used is restricted to the stability condition as mentioned in equation (17):

$$\left[\frac{D\Delta t}{(\Delta x)^2} + \frac{D\Delta t}{(\Delta y)^2} \right] \leq \frac{1}{2} \quad (17)$$

3. Results and discussion

3.1 Verification of ADI method

The comparison of the ADI method with the semi-analytical method is illustrated in figure 2. The ADI approximation agrees well with the semi-analytical solution. Next, the verified ADI method is implemented to estimate the carbon concentration profile within the carbon steel 1024 during carburisation process.

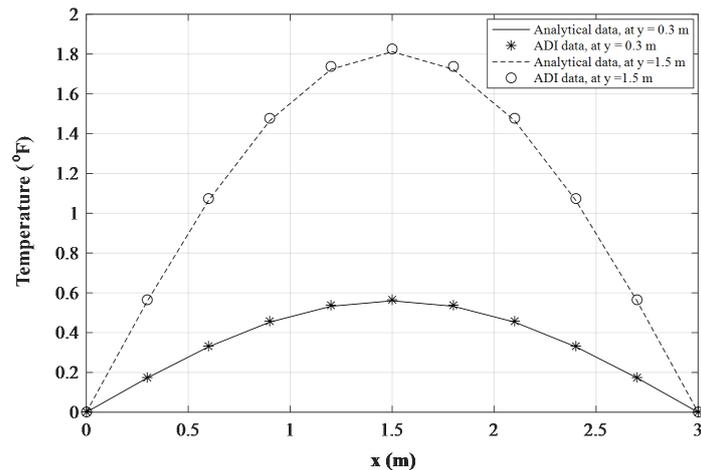
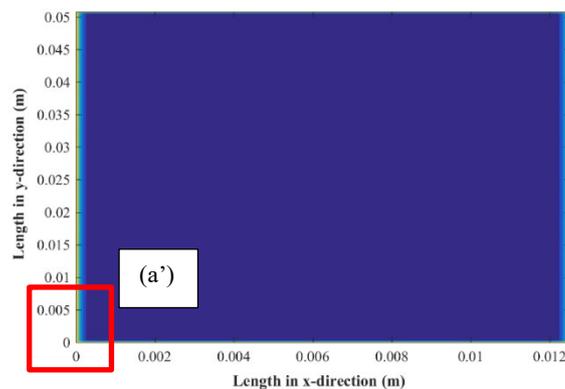


Figure 2. Temperature distribution for the heat conduction problem along x-axis at $y = 0.3$ m and $y = 1.5$ m for 1.2 hr.

3.2 Prediction of carbon concentration profile within the carbon steel 1024 structure during pack carburisation

The contour plot of the carbon concentration profile for carburised- carbon steel after 3 hours of reaction in figure 3(a) displays a very small changes near the sample surface. This is common in carburisation process, where the main focus of the treatment is to increase the carbon content within the case or certain depth below the steel surface, not the core of the steel. In each direction, carbon concentration progressively slow as depicted in figure 3(b). Hence, for clearer image, the discussion is focused on the optimum depth of 0.0015m as shown in figure 3(c).



(a)

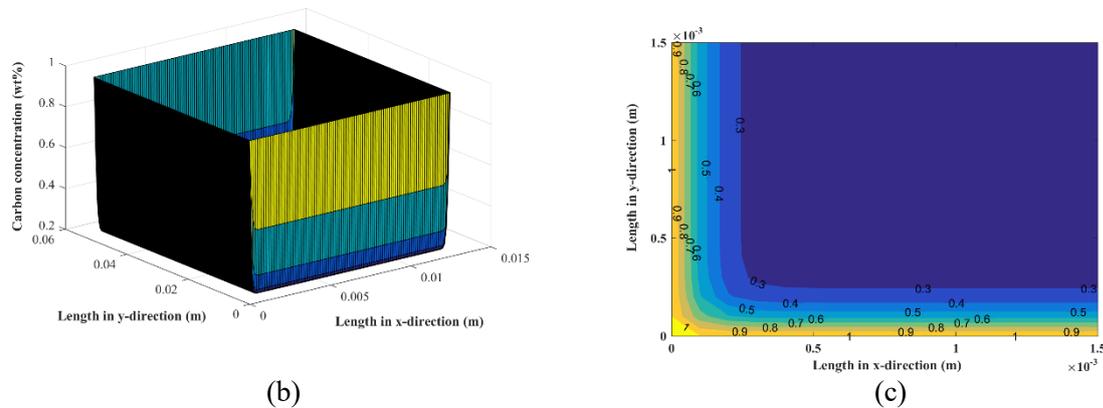


Figure 3. Simulation results of carburisation at 900°C for 2 hours (a) Overall contour plot of carbon steel; (b) Surface plot of carbon concentration profile; (c) Enlarged image of contour plot (a') at the corner of the carbon steel in x and y direction.

3.3 Effect of carburisation time

The carburisation time is varied from 2 hours to 60 hours. The development of carbon concentration within the carbon steel are illustrated by contour plots in figure 5. The core of the carbon steel constantly having 0.3 wt% of carbon content with its surface slowly penetrated by the diffused carbon over time.

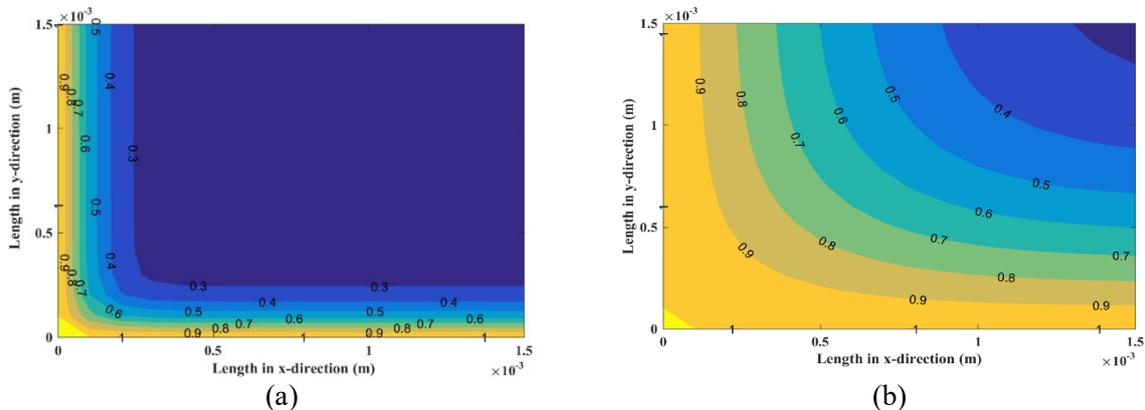


Figure 4. Contour plot of carbon concentration within the carbon steel at various carburising time; (a) 2 hours; 60 hours.

Figure 5 shows a closer look on the dynamic of carbon diffusion at 0.0015 m, the optimum depth from each dimension surface. It is interesting to note that the simulated result for carbon concentration of carburisation for 3 hours can explain the case depth of carbon steel conducted by Ali et al., 2016 [1]. The measured case depth is 0.468×10^{-3} m which comparable with the simulated carbon concentration profile in this study.

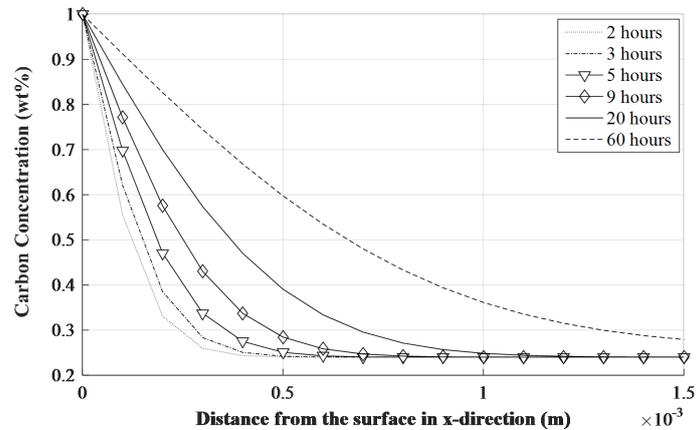
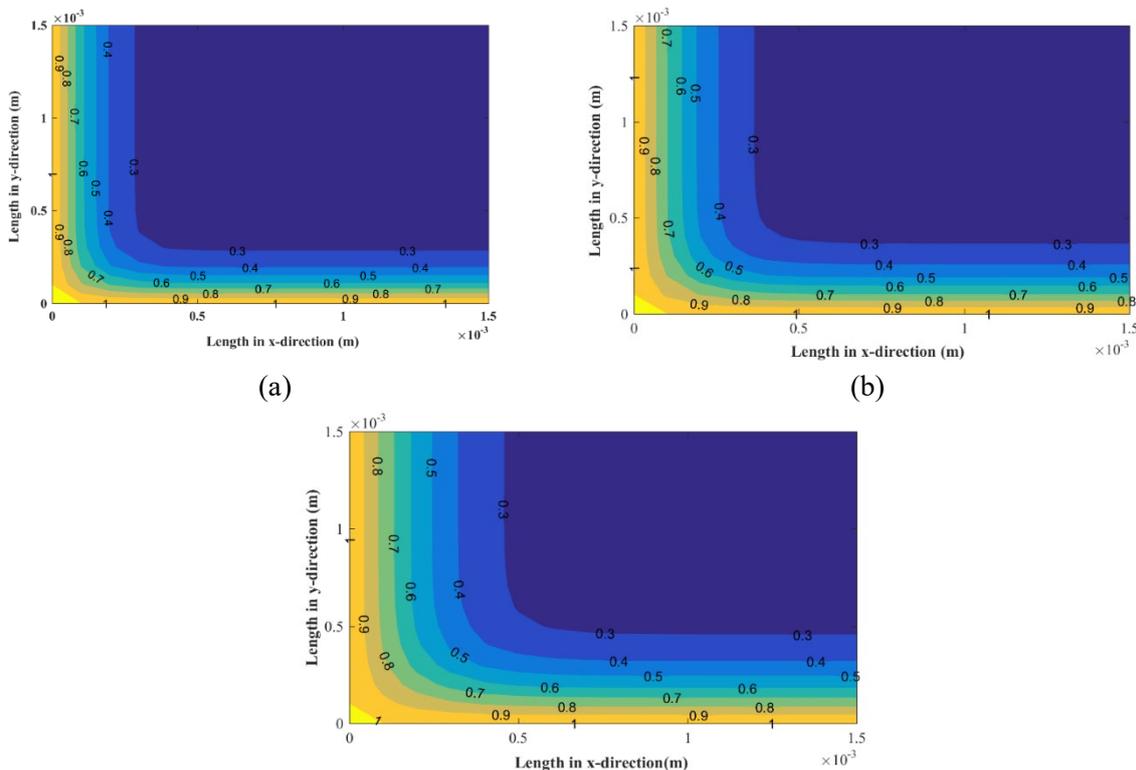


Figure 5. Carbon concentration profile at optimum depth of 0.0015 m from the carbon steel surface carburised at 2 hours, 3 hours, 5 hours, 9 hours, 20 hours and 60 hours in x direction along $y = 0.0015$ m.

Increasing the carburising time will ensure the increment of diffused carbon for both directions. This is due to the continuous decomposition of CO_2 gas and BaCO_3 . At 2 hours of reaction, more carbon atoms enter the structure of steel. Thus, the rate of diffusion is also increases. But after some time, less carbon atoms remained in the pack. Therefore, the carbon diffusion eventually slow [12].

3.4 Effect of carburisation temperature

The carbon steel is simulated with three different carburisation temperature of 900°C, 950°C and 1000°C for 3 hours. Figure 6 shows contour plots of carbon concentration within the carburised- carbon steel. The carbon content is increasing with carburisation temperature.



(c)

Figure 6. Contour plots of carbon concentration within 3 hours carburised- steel at carburising temperature of (a) 900°C; (b) 950°C; (c) 1000°C

The region contains 0.3 wt% becoming smaller as carbon diffuses within the structure. This is because of increases in the flux of carbon atoms due to the positive influence of the carbon diffusion coefficient D with the temperature of carbon steel. Higher temperatures provide sufficient thermal energy to the diffusing carbons that overcome the activation energy barrier and facilitate their movement to new sites in atomic arrangements. The graphical representation of the carbon concentration at the optimum depth of 0.0015 m below the surface of x and y dimension as illustrated in figure 7 shows that the rapid changes can be made by extending the carburisation duration time and increasing the temperature.

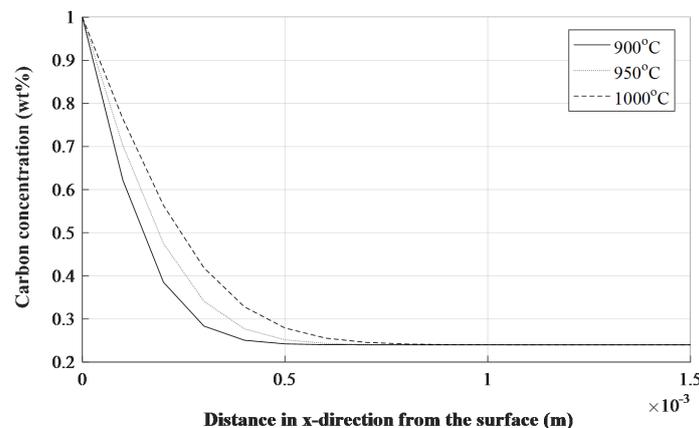


Figure 7. Carbon concentration profile at optimum depth of 0.0015 m from the carbon steel surface carburised at 900°C, 950°C and 1000°C in x -direction along $y=0.0015$ m.

4. Conclusion

The transient two-dimensional diffusion equation has been discretised using ADI method and the numerical algorithm in MATLAB has been successfully verified analytically. As a results, prediction of carbon concentration profile within the carburised-carbon steel is efficaciously visualised using various representations. Simulation results show that carburisation extended to 60 hours only increases the carbon content at the core to 0.3wt % from its original content which is 0.24 wt%. The small increment is required to maintain its ductility even though the surface is hardened. The developed ADI method can be used to solve engineering process involve transient two dimensional parabolic equation such as mass diffusion and heat conduction.

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