Modeling LHP in carbon steel-1045 during quenching

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Abstract

The modelling of an axisymmetric industrial quenched carbon steel-1045 based on finite element method has been produced to investigate the impact of process history on metallurgical and material properties. Mathematical modelling of 1-Dimensional line (radius) element axisymmetric model has been adopted to predict temperature history and consequently the hardness of the quenched steel bar at any point (node). The lowest hardness point (LHP) is determined. In this paper hardness in specimen points was calculated by the conversion of calculated characteristic cooling time for phase transformation t8/5 to hardness. The model can be employed as a guideline to design cooling approach to achieve desired microstructure and mechanical properties such as hardness. The developed mathematical model converted to a computer program. This program can be used independently or incorporated into a temperature history software which named LHP-software to continuously calculate and display temperature history of the industrial quenched steel bar and thereby calculate LHP. The developed program from the mathematical model has been verified and validated by comparing its hardness results with experimental work results. The comparison indicates reliability of the proposed model.

Keywords:, Heat Treatment; Quenching; Axisymmetric Chromium Steel Bar; Finite Element; Mathematical Modeling; Unsteady State Heat Transfer.

1. Introduction

Quenching of steels is a multi-physics process involving a complicated pattern of couplings among heat transfer. Because of the complexity, coupled (thermal-mechanical-metallurgical) theory and non-linear nature of the problem, no analytical solution exists. However, numerical solution is possible by finite difference method, finite volume method, and the most popular one - finite element method (FEM). During the quenching process of the steel bar, the heat transfer is in an unsteady state as there is a variation of temperature with time.

In this paper the heat transfer analysis will be carried out in 3- dimensions. The three dimensional analysis will be reduced into a 1-dimensional axisymmetric analysis to save cost and computer time. This is achievable because in axisymmetric conditions, the temperature deviations is only in (R) while there is no temperature variation in the theta (Θ) and (Z) direction as it is clear in Fig. 1, Fig. 2 and Fig. 3. The Galerkin weighted residual technique is used to derive the mathematical model.

In this work, 1-Dimensional line (radius) element will be developed to determine LHP, water cooled.

2. Mathematical model

The temperature history of the quenched cylindrical carbon steel-1045 bar at any point will be calculated. Three dimensional heat transfers can be analyzed using one dimensional axisymmetric element as shown in Fig. 1, Fig 2 and Fig 3.

2.1 Methodology of building the F. E. Model in details

The temperature distribution inside the cylindrical steel bar when reached thermal equilibrium will be calculated. These are special classes of three-dimensional heat transfer problem:

- i. Geometrically axisymmetric.
- ii. Each thermal load is symmetrical about an axis.

This three-dimensional heat transfer problem may be analyzed using one-dimensional axisymmetric elements as shown in Figs. 1, Fig. 2 and Fig. 3.

The finite element method is applied to the one-dimensional cylindrical coordinates heat transfer problem. The finite element formulation is developed with the Garlekin Weighted-residual method. The appropriate working expressions of the conductance matrix, capacitance matrix and thermal load matrix are derived in details.

The time dependent solution is obtained by applying the Backward Difference Scheme [BDS].

2.1.1 Meshing the engineering problem of the domain

Meshing of the domain according to which kind of element selected, where our research is one-dimensional axisymmetric elements then line element have been selected on this mathematical model. Let us consider a cylindrical carbon steel-1045 bar as shown in Fig. 1 which had been heated and then submerged in water.

The linear temperature distribution for an element (radius) line, T is given by:

$$T^{(R)} = a_1 + a_2 R$$
 (1)

Where,

 $T^{(R)}$ = nodal temperature as the function of R, a_1 and a_2 are constants. R is any point on the (radius) line element.

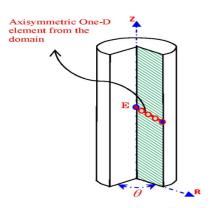


Figure 1: The axisymmetric one dimensional line (radius) element from the domain, on the cylindrical carbon steel 1045 which had been heated and then

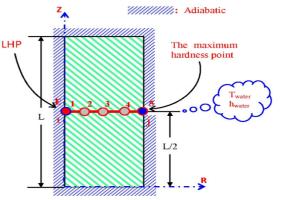


Figure 2: The axisymmetric one dimensional line

(radius) element From the domain on the

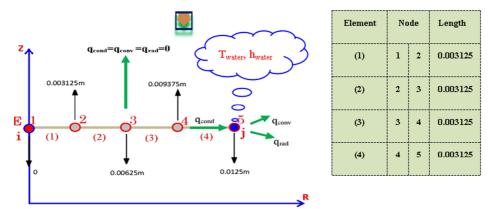


Figure 3: The axisymmetric one dimensional line (radius) element from the domain, the selected 4 elements with 5 nodes and the boundary at node j [5] for an element 4.

2.1.2 Shape function of 1-D axisymmetric element

The shape functions were to represent the variation of the field variable over the element. The shape function of axisymmetric 1-Dimensional line (radius) element expressed in terms of the r coordinate and its coordinate are shown in Fig. 4;

$$S_{i} = \left(\frac{R_{j} - R_{j}}{R_{j} - R_{j}}\right) = \left(\frac{R_{j} - R_{j}}{L}\right)$$
(2a)

$$S_{i} = \left(\frac{R - R_{i}}{R_{i} - R_{i}}\right) = \left(\frac{R - R_{i}}{L}\right)$$
(2b)

Thus the temperature distribution of 1-D radius for an element in terms of the shape function can be written as:

$$T^{(R)} = S_i T_i + S_j T_j = S^{(r)} \{T\}$$
(3)

Where, $[S^{(r)}] = [S_i \quad S_i]$ is a row vector matrix and

 $\{T\}$ = is a column vector of nodal temperature of the element.

Eq. (3) can also be expressed in matrix form as:

$$\mathbf{T}^{(\mathbf{R})} = \begin{bmatrix} \mathbf{S}_{i} & \mathbf{S}_{j} \end{bmatrix} \begin{cases} T_{i} \\ T_{j} \end{cases}$$
(4)

Thus for 1-dimensional element we can write in general:

$$\Psi^{(e)} = \begin{bmatrix} S_i & S_j \end{bmatrix} \begin{cases} \psi_i \\ \psi_j \end{cases}$$
(5)

Where Ψ_i and Ψ_j represent the nodal values of the unknown variable which in our case is temperature.

The unknown can also be deflection, or velocity etc.

2.1.3 Natural area coordinate

Using the natural length coordinates and their relationship with the shape function by simplification of the integral of Galerkin solution:

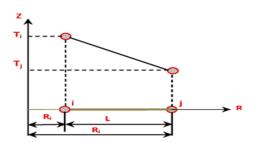


Figure 4: One-dimensional linear temperature distribution for an element (radius) line in Global Coordinate system.

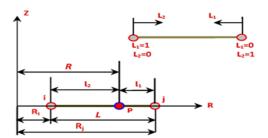


Figure 5: Two-node line element showing interior point p and the two naturals coordinates L_1 and L_2 .

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The two length natural coordinates L_1 and L_2 at any point p inside the element are shown in Fig. 5 from which we can write:

$$L_{1} = \frac{R_{j} - R_{i}}{R_{j} - R_{i}} = \frac{l_{1}}{L}$$
(6a)
(6b)
(6b)

Since it is a one-dimensional element, there should be only one independent coordinate to define any point P. This is true even with natural coordinates as the two natural coordinates L_1 and L_2 are not independent, but are related as:

 $L_1 + L_2 = S_i + S_j = 1$

2.2 Develop Equation for all Elements of the Domain

Derivation of equation of heat transfer in axisymmetric one-dimensional line (radius) elements by applying the conservation of energy to a differential volume cylindrical segment has been done. As shown in Fig. 6;

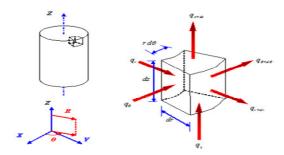


Figure 6: Axisymmetric element from an axisymmetric body.

$$E_{in} - E_{out} + E_{generated} = E_{stored}$$
(7)

The transient heat transfer within the component during quenching can mathematically be described by simplifying the differential volume term; the heat conduction equation is derived and given by;

$$\frac{1}{r}\frac{d}{dr}\left(K_{r}r\frac{dT}{dr}\right) + \frac{1}{r^{2}}\frac{d}{d\theta}\left(K_{\theta}\frac{dT}{d\theta}\right) + \frac{d}{dz}\left(K_{z}\frac{dT}{dz}\right) + q = \rho c\frac{dT}{dt}$$

$$\tag{8}$$

 k_r = heat conductivity coefficient in *r*-direction, W/m·°C, k_{θ} = heat conductivity coefficient in θ -direction, W/m·°C. kz = heat conductivity coefficient in *z*-direction, W/m·°C, *T* = temperature, °C, *q* = heat generation, W/m³,

 ρ = mass density, kg/m³. c = specific heat of the medium, J/kg·K and t = time, s.

2.3 The assumption made in this problem was:

- i. For axisymmetric situations one dimensional line (radius) element, there is no variation of temperature in the Zdirection as shown in Figs. 1, Fig. 2 and Fig. 3. Therefore we can write, $\left(\frac{\partial T}{\partial z} = 0\right)$
- ii. For axisymmetric situations, there is no variation of temperature in the θ -direction, because it is clear from Figs. 1, Fig. 2 and Fig. 3 that the temperature distribution along the radius will be the same if the radius move with angle θ , 360°. Therefore, $\left(\frac{\partial T}{\partial \theta} = 0\right)$
- iii. The thermal energy generation rate \dot{q} represents the rate of the conversion of energy from electrical, chemical, nuclear, or electromagnetic forms to thermal energy within the volume of the system, however in this manuscript no heat generation has been taken into accounted. Therefore, $\dot{q} = 0$

After simplifying, Eq. (8) becomes;-

$$\frac{k}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) = \rho \ c\frac{\partial T}{\partial t}$$
(9)

And also known as residual or partial differential equation

$$\left\{\mathfrak{R}\right\} = \frac{k}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) - \rho \ c\frac{\partial T}{\partial t} = 0$$
(10)

2.4 Galerkin Weighted Residual Method Formulation

From the derived heat conduction equation, the Galerkin residual for 1-dimensional line (radius) element in an unsteady state heat transfer can be obtained by integration the transpose of the shape functions times the residual which minimize the residual to zero becomes;

$$\int_{V} [S]^{T} \left\{ \mathfrak{R} \right\}^{(e)} dv = 0 \tag{11}$$

Where, $[S]^{T}$ = the transpose of the shape function matrix and $\{\Re_{R_{i}}\}^{(e)}$ = the residual contributed by element (e) to the final system of equations.

After derivation, simplification and rearranged, we get:



$$= \underbrace{\overline{k}}_{r} \int \left\{ \frac{\partial}{\partial r} \left(\left[S \right]^{T} r \frac{\partial T}{\partial r} \right) \right\} dv - \underbrace{\overline{k}}_{r} \int \left\{ \frac{\partial \left[S \right]^{T}}{\partial r} r \frac{\partial T}{\partial r} \right\} dv - \underbrace{\int \left[S \right]^{T} \left\{ \rho c \frac{\partial T}{\partial t} \right\} dv}_{C}$$
(12)

Term A is the heat convection terms and contributes to the conductance and thermal load matrix.

Term B is the heat conduction terms and contributes to the conductance matrix. Term C is the transient equation and contributes to the capacitance matrix.

Finally we can formulate the conductance matrix in the r-direction for term A, B and term C, we get:

Term A (Heat Convection):

Term A₁ (the convection term) contributes to the conductance matrix:

$$\begin{bmatrix} 2 & hR \\ - 2 & hR \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} Ti \\ Tj \end{bmatrix}$$

$$(13)$$

 $\mathbf{K}_{\mathbf{h}}$

Term A₂ (the convection term) contributes to thermal load matrix:

$$2 h R_{j} T_{w} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$
(14)

Term B (the conduction term) contributes to the conductance matrix:

$$\frac{k}{L} \begin{pmatrix} R \\ j \end{pmatrix} + \begin{pmatrix} R \\ i \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} T_i \\ T_j \end{pmatrix} \begin{bmatrix} T_i \\ T_j \end{bmatrix}$$
(15)

 f_h

Term C (heat stored) contributes to the Capacitance Matrix:

$$\begin{bmatrix}
\underline{L \ \rho \ c} \\
6
\end{bmatrix}
\begin{bmatrix}
\begin{pmatrix}
3 \ R_{\ i} + R_{\ j} \\
R_{\ i} + R_{\ j}
\end{pmatrix}
\begin{bmatrix}
\overline{T}_{\ i} \\
T_{\ j}
\end{bmatrix}
\begin{bmatrix}
\overline{T}_{\ i} \\
T_{\ j}
\end{bmatrix}$$
(16)

2.5 Construct the element Matrices to the Global Matrix

The global, conductance, capacitance and thermal load matrices and the global of the unknown temperature matrix for all the elements in the domain are assembled i.e. the element's conductance; capacitance and thermal load matrices have been derived. Assembling these elements is necessary in all finite element analysis.

Constructing these elements will result into the following finite element equation:

$$[K]^{(G)} \{T\}^{(G)} + [C]^{(G)} \{\dot{T}\}^{(G)} = \{F\}^{(G)}$$
(17)

Where: $[K^{](G)} = [K_c] + [K_h]$: is conductance matrix due to Conduction (Elements 1 to 4) and heat loss through convection at the element's boundary (element 4 node 5) as shown in Figs. 1, Fig. 2 and Fig. 3, {T}: is temperature value at each node, °C, [C]: is capacitance matrix, due to transient equation (heat stored) and {T}: is temperature rate for each node, °C/s.

 ${F}^{(G)} = {F_h} + {F_q}$: is heat load due to heat loss through convection at the element's boundary (element 4 node 5) and internal heat generation (element 4 node 5).

2.6 Euler's method

Two point recurrence formulas will allow us to compute the nodal temperatures as a function of time.

In this paper, Euler's method which is known as the backward difference scheme (FDS) will be used to determine the rate of change in temperature, the temperature history at any point (node) of the steel bar. If the derivative of T with respect to time t is written in the backward direction and if the time step is not equal to zero ($\Delta t \neq 0$), we have;

$$\left\{ \dot{\mathbf{T}} \right\} \approx \left\{ \frac{T(t) - T(t - \Delta t)}{\Delta t} \right\}$$
(18)

With; \dot{T} = temperature rate (°C/s); T (t) = temperature at t s (°C); T (t- Δt) = temperature at (t- Δt) s, (°C), Δt = selected time step (s) and t = time (s) (at starting time, t = 0), By substituting { \dot{T} } into the finite element global equation, we have that;

 $[K]^{(G)} \{T(t)\}^{(G)} + [C]^{(G)} \{\frac{T(t) - T(t - \Delta t)}{\Delta t}\}^{(G)} = \{F(t)\}^{(G)}$ ⁽¹⁹⁾

Finally, the matrices become;

$$\left[\left[K \right]^{(G)} \Delta t + \left[C \right]^{(G)} \right] \left\{ T \right\}_{i+1}^{(G)} = \left[C \right]^{(G)} \left\{ T \right\}_{i}^{(G)} + \left\{ F \right\}_{i+1}^{(G)} \Delta t$$
(20)

From Eq. (20) all the right hand side is completely known at time t, including t = 0 for which the initial condition apply. Therefore, the nodal temperature can be obtained for a subsequent time given the temperature for the preceding time. Once the temperature history is known the important mechanical properties of the carbon steel-1045 can be obtained such as hardness and strength.

3. APPLICATION

3.1 Calculation the temperature history

The present developed mathematical model is programmed using MATLAB to simulate the results of the temperature distribution with respect to time in transient state heat transfer of the industrial quenched carbon steel-1045. The cylindrical carbon steel-1045 bar has been heated to 850°C. Then being quenched in water with $T_{water} = 32^{\circ}C$ and the convection heat transfer coefficient, $h_{water} = 5000 \text{ W/m}^2 \cdot \text{C}$.

The temperature history for the selected nodes of the cylindrical carbon steel-1045 bar when the radius = 12.5 mm after quenching is being identified in Fig. 7 and Fig. 8. The cylindrical bar was made from carbon steel-1045, with properties as mentioned below:

Density = 7872 kg/m3

Specific heat = 486 J/Kg.K

Thermal capacity, $\rho c (J/m3 \cdot {}^{\circ}C)$.

 $0 \le T \le 650$ °C, $\rho c = (0.004 T + 3.3) \times 10^{-6}$ 650 < $T \le 725$ °C, $\rho c = (0.068 T - 38.3) \times 10^{-6}$

725 < T ≤ 800 °C, $\rho c = (-0.086 T + 73.55) \times 10^{-6}$, T > 800 °C, $\rho c = 3.825792 \times 10^{-6}$

Thermal conductivity, $k (W/m^{\circ}C)$: $0 \le T \le 900 {}^{\circ}C, k = -0.022 T + 48 T > 900 {}^{\circ}C, k = 50.9$

In our case Eq. 20 becomes:

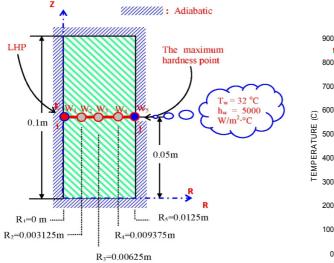
 $[K]^{(G)} \{T\}^{(G)} + [C]^{(G)} \{T\}^{(G)} = \{F\}^{(G)}$ and their respective equation;

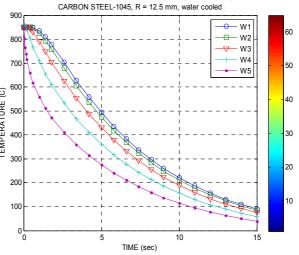
$$[K]^{(G)} = [K_c]^{(1)} + [K_c]^{(2)} + [K_c]^{(3)} + [K_c]^{(4)} + [K_h]^{(4)}$$
(21)

$$\begin{bmatrix} C \end{bmatrix}^{(G)} = \begin{bmatrix} C \end{bmatrix}^{(1)} + \begin{bmatrix} C \end{bmatrix}^{(2)} + \begin{bmatrix} C \end{bmatrix}^{(3)} + \begin{bmatrix} C \end{bmatrix}^{(4)}$$
(22)

$$\{F\}^{(G)} = \{F_h\}^{(4)} \tag{23}$$

With the input data and boundary conditions provided, a sensitivity analysis is carried out with the developed program [LHP-software] to obtain the temperature distribution at any point (node) of the quenched steel bar. As an example the transient state temperature distribution results of the selected five nodes from the center $[W_1]$ to the surface $[W_5]$ of the quenched carbon steel-1045 bar which were computed are shown in Fig. 7 and Fig. 8.





TEMPERATURE HISTORY OF THE SELECTED 5 NODES

Figure 7: The axisymmetric one dimensional line (radius) element from the domain, the selected 4 elements with 5 nc and the boundary at node j [5] for an element 4.

Fig. 8 Graph of temperature history along WW cross-section when the radius equal 12.5 mm from LHP-software.

3.2 LHP Calculation

3.2.1 Calculating the cooling time required

As known during quenching, there are two important temperatures [$800^{\circ}C$ and $500^{\circ}C$] to calculate the cooling time, because the characteristic cooling time, relevant for structure transformation for most structural steels, is the time of cooling from 800 to 500°C (time t_{8/5}).

$t_c = t_{800} - t_{500}$

From Fig. 8 when the radius = 12.5mm we can determine the time taken for node W_1 to reach 800°C, and the time taken for node W_1 to reach 500°C.

So the Cooling time t_c for node W_1 ;

 $t_c = t_{800}$ - $t_{500} = 3.381020$ sec

For nodes W₂ to W₅, the cooling time t_c calculated by the same way, the final results shown in Table 1.

3.2.2 Calculating the Jominy distance from Standard Jominy distance versus cooling time curve

Cooling time, t_c obtained will now be substituted into the Jominy distance versus cooling time curve to get the correspondent Jominy distance. Jominy distance can also be calculated by using polynomial expressions via polynomial regression via Microsoft Excel.

The standard Table [Cooling rate at each Jominy distance (Chandler, H., 1998)] can be used too.

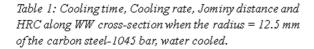
Then Jominy distance of nodes W₁ to W₅ will be calculated, the final results shown in Table 1, where:

The Rate of Cooling, ROC, was defined by;

ROC = $\frac{800 \text{ °C} - 500 \text{ °C}}{t_c} = \frac{800 \text{ °C} - 500 \text{ °C}}{t_{500 \text{ °C}} - t_{800 \text{ °C}}} (\text{ °C/s})$

3.2.3 Predict the hardness of the quenched steel bar

The HRC can be calculated by using the relation between the J-Distance and the HRC as explained in section 3.2.2, the final results shown in Table 1, Fig. 9:



Node	te (s)	ROC (°C/s)	J-distance mm	HRC
W1	3.38102	88.7306	5.386	41.956
W2	3.34327	89.7325	5.347	42.112
W3	3.14244	95.4672	5.141	42.936
W4	2.58465	116.0699	4.467	44.300
W 5	1.46664	204.5492	2.457	53.039

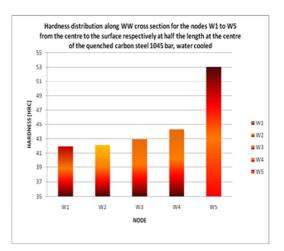


Fig. 9 Hardness distribution along WW cross section of the quenched carbon steel-1045 bar, water cooled.

4. Mathematical model verification

Where, the lowest hardness point can be determined by developing mathematical model, but it is impossible to calculated by experimental work, therefore the developed mathematical model has been verified by calculating the hardness on the surface, for both mathematical model and experimentally, however a strong agreement between both results conformed so thereby this served as a validated to the experiment, the comparison got across that the reliability of the proposed model indicated that the calculation of the lowest hardness point at is correct. Where, it was found as shown in Fig. 9 that the hardness at the surfaces node $[W_5]$ equal 53.039 by developed 1-D mathematical model. And it was found that the average hardness at the same node on the surface $[W_5]$ equal 52.607 by experimental work.

5. DISCUSSIONS AND CONCLUSION

A 1-D mathematical model of transient industrial quenched carbon steel-1045 has been developed to compute the temperature distribution in specimens with a cylindrical geometry to determine LHP.

It is clear from our results that the nodes on the surfaces cool faster than the nodes at half the length at the centre because t_c of node W_5 less than t_c of node W_1 as shown in Fig. 8.

This means that the mechanical properties such as hardness will be different. Where the hardness on the surface node will be higher than the hardness on the center the results showed that the node on the surface will be the first to be completely cooled after quenching.

Because it is in the contact with the cooling medium then the other points (nodes) on the radial axis to the centre respectively while the last point that will be completely cooled after quenching will be at half the length at the centre that is LHP node W_1 shown in Fig. 9.

Experimental calculation of LHP is an almost impossible task using manual calculation techniques. Also the earlier methods only used hardness calculated at the surface, which is higher than LHP, which has negative consequence and can result in the deformation and failure of the component.

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