Microstructure simulation during quenching

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1. INTRODUCTION

Quenching is a commonly used heat treatment process employed to control the mechanical properties of steels. Induction hardening with quenching is one of the most common industrial hardening process of steels. In IKERLAN it's a new initiation to consider the residual stresses from hardening of steel components for fatigue and crack analysis. Simulation options of Induction hardening is not readily available in the commercial software packages available in IKERLAN, such as ANSYS and FLUX. An effort to implement Induction hardening in these available software packages is a challenging task, especially the microstructure simulation. The goal of the simulation model is to calculate the residual stress field of the analyzed component and for this aim it is essential to consider microstructure simulation.

For cost efficiency, it's required to consider available commercial or open source software for simulation. For structural analysis Code Aster is a good open source software and it also has provision for Microstructure simulation. Apart from open source software packages, there is a provision for implementing missing configurations in ANSYS through coding in APDL (Ansys Parametric Design Language). In this study, possible options for microstructure simulation are considered.

2. LITERATURE REVIEW

Quenching simulation consists of complex process. In this process the various domains are coupled as shown in figure 1 ,
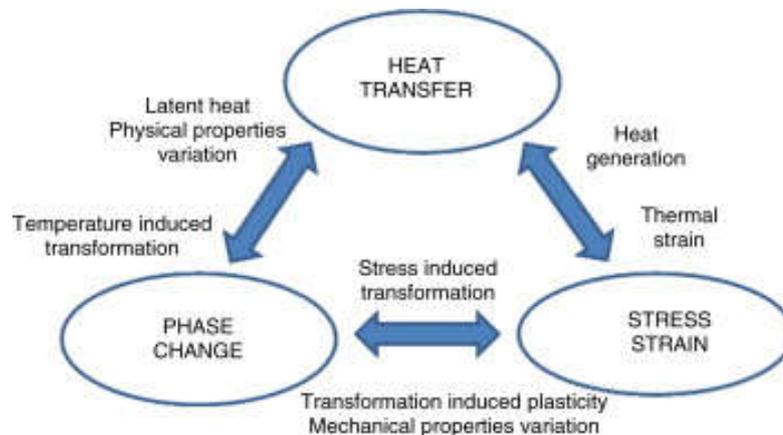

Figure 1. Metallographic, thermal, and mechanical coupling effects in the quenching process [1].

There are three main two-way couplings.

1) Thermal-Mechanical

2) Metallurgical-Mechanical

3) Thermal-Metallurgical

Metallurgical or microstructure simulations are not implemented in most of commercial general purpose or structural FEM software packages.

Metallurgical Simulations are categorized in to two types,

1) Isothermal model simulation

2) Non-isothermal model simulation

Most of the available literature is on Isothermal model and no algorithm or equations are available for highly non-isothermal process like quenching. From literature review, an effort is made to simply the concepts and algorithms.

1) Isothermal model simulation: Isothermal simulations are valid for isothermal cooling in furnaces or cooling in salt baths. This model uses TTT diagram (IT diagrams). TTT diagram of Steel 42CrMo4 is shown in figure 1a (from ref. 8).The transformation results in any of the four microstructures namely Ferrite, Pearlite, Bainite and Martensite. The governing equations for diffusional transformation such as Astenite to Ferrite, Astenite to Pearlite and Astenite to Baininte is Avrami (JMAK) equation is given by,

$$F_i(T) = 1 \quad \exp[\quad a(T) \quad t(T)^{n(T)}]$$

Where F_i is the volume fraction of the product phase i, t is the time elapsed since the transformation beginning, i.e. after the nucleation process, a and n are material parameters, dependent on the isothermal temperature and the forming phase. The diffusional coefficient a and the transformation exponent n can be evaluated by the IT diagram of the considered material, taking into account the time τ_s and τ_f needed for the conversion, in isothermal conditions, of detectable start and finish volume fractions, indicated, respectively, as F_s and F_f, of the forming phase, as follows:

$$a(T) = \quad \ln(F_s)\tau_s(T)^{-n(T)}$$

$$n(T) = \frac{\ln(\ln(F_f) \quad \ln(F_s))}{\ln(\tau_s(T)) \quad \ln(\tau_f(T))}$$

Where the subscripts s and f refer to the starting and finishing conditions of the phase change. In the present investigation F_s and F_f have been assumed, respectively, as 0.01 and 0.99. The discretized equations are available in reference 1 and 7.

A sample code is available based on this equation which is discussed on later sections (from ref.2).
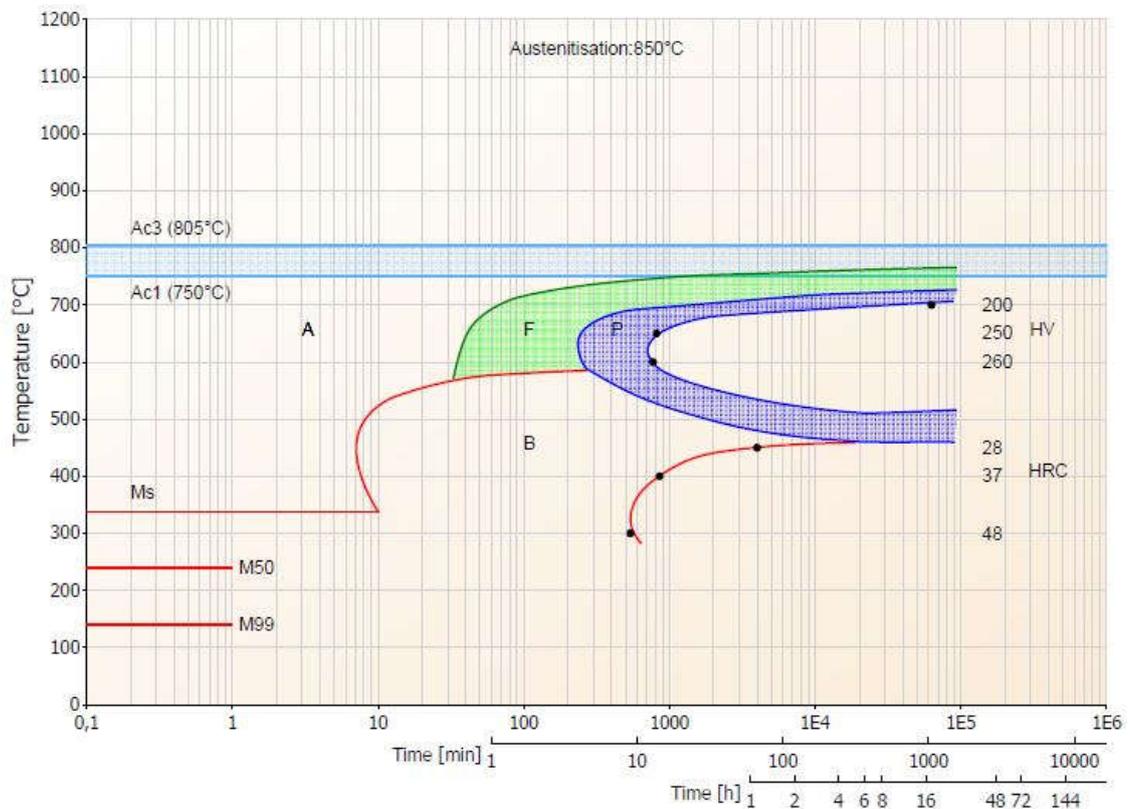

Figure 1a. TTT diagram of Steel 42CrMo4

2) Non-isothermal model simulations: This is most suitable model for quenching. Quenching involves rapid cooling, hence it is highly non-isothermal. Owing to the complexity of this metallurgical process no equations are readily available. However, using Continuous Cooling Diagram (CCT) diagrams simulations are carried in sophisticated metallurgical software packages [2]. CCT diagram of Steel 42CrMo4 is shown in figure 1b (from ref. 8).
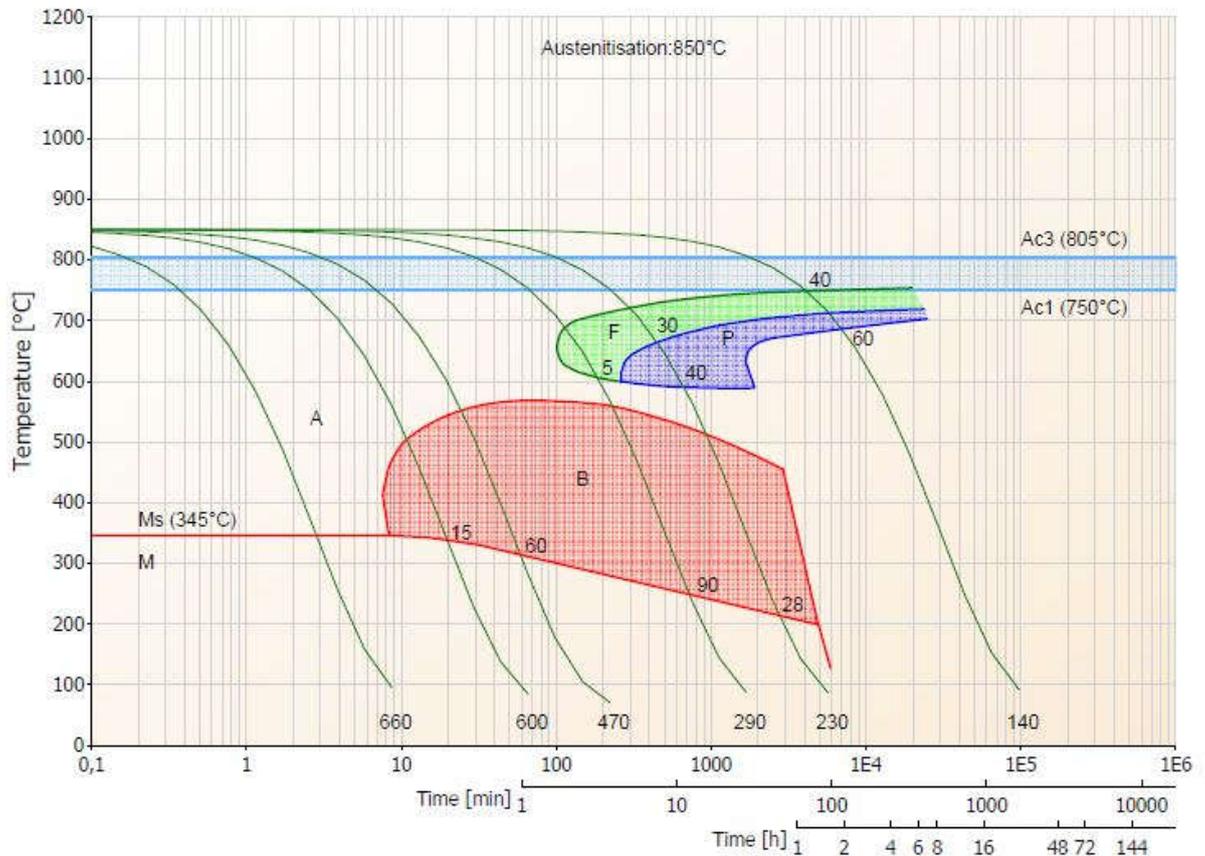

Figure 1b. CCT diagram of Steel 42CrMo4

ANSYS and Code Aster software mainly considered for implementing these microstructure models for quenching. Commercial available software packages at IKERLAN are ANSYS and FLUX. It is economical to implement missing aspects to these software to achieve Induction hardening simulation. Code Aster is one of the main open source software for FEM and structural analysis. It has some part of microstructure simulation implemented [3, 4 & 5]. Hence, Code Aster and ANSYS APDL are considered for micro-structure simulation.

3. CODE ASTER FOR MICROSTRUCTURE SIMULATION

In code Aster most of the codes and documentations are freely available. For quenching documentations and sample codes are available for isothermal model. The algorithm and important code words are available in code Aster documents U2.03.04, R4.04.01 and R4.04.02 (ref. 3, 4 & 5).

Some of the important code words for isothermal simulation are,
CALC_META - Operator to obtain hardness of the multiphase mixture.
DEFI_TRC - defines the evolutions of Ferrite, Pearlite and Bainite associated with a set of thermal history.
CREA_CHAMP - Definition of the initial Metallurgical Phases
DEFI_MATERIAU – To define material properties
META_ECRO_LINE - To define an Isotropic or Kinematic Work Hardening

In reality, quenching is highly non isothermal process and hence isothermal algorithm is being made to fit into quenching. Few groups of researchers are working on this [9 & 10].

Code Aster is French software and its parametric codes are from French origin. This coding language has no relation with ANSYS APDL. Hence, code Aster cannot fulfill the microstructure requirement of ANSYS. Only, ANSYS APDL can be used for that purpose. However, Code Aster can be used with FLUX software to perform induction hardening simulation.

A simulation flow chart for Gear Teeth is shown in fig. 2 (from ref. 6). The electromagnetic simulation and thermal simulation is carried out in Flux software and the results are exported through flux python. These results are to be conveniently fed to Code Aster for further analysis. Hence, interpolation of temperature heating nodal evaluation on code Aster mesh is carried out using MATLAB. Then, using Python the interpolated data is saved in MED format with MED Coupling and MED Loader Libraries. Using these MED inputs the quenching simulation is carried out in Code Aster (Salome Meca) and the residual stresses are evaluated.
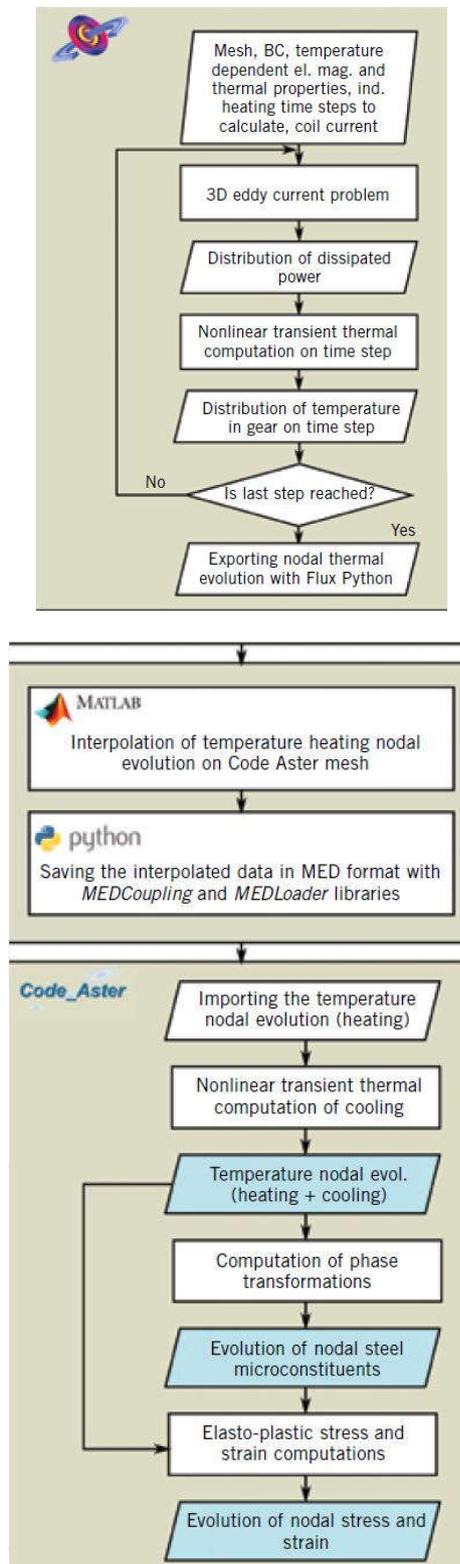
Fig. 2 Simulation flow chart of Induction hardening using FLUX and Code Aster

4. MICROSTRUCTURE SIMULATION USING APDL

ANSYS APDL is considered for microstructure simulation. Initially a 2D model or steel plate is considered as shown in figure 3. Arbitrary conditions are applied. The right edge is quenched with water (h_1 = 10000 W/m²) and other three sides are exposed to air at atmospheric temperature (h_2 = 25 W/m²). Initial temperature of plate is 850° C. Ambient air temperature is 25° C. Transient thermal analysis is carried out in ANSYS APDL (Classic). The temperature distribution after 10s is shown in figure 4. It can be observed that the temperature is minimum at the quenched edge. Microstructure simulation is carried out using APDL commands. Martensitic fraction is evaluated using linear dependency on temperature. It is given by,

$$F(T_i) = \frac{(T_i \quad M_s)}{(M_f \quad M_s)}$$

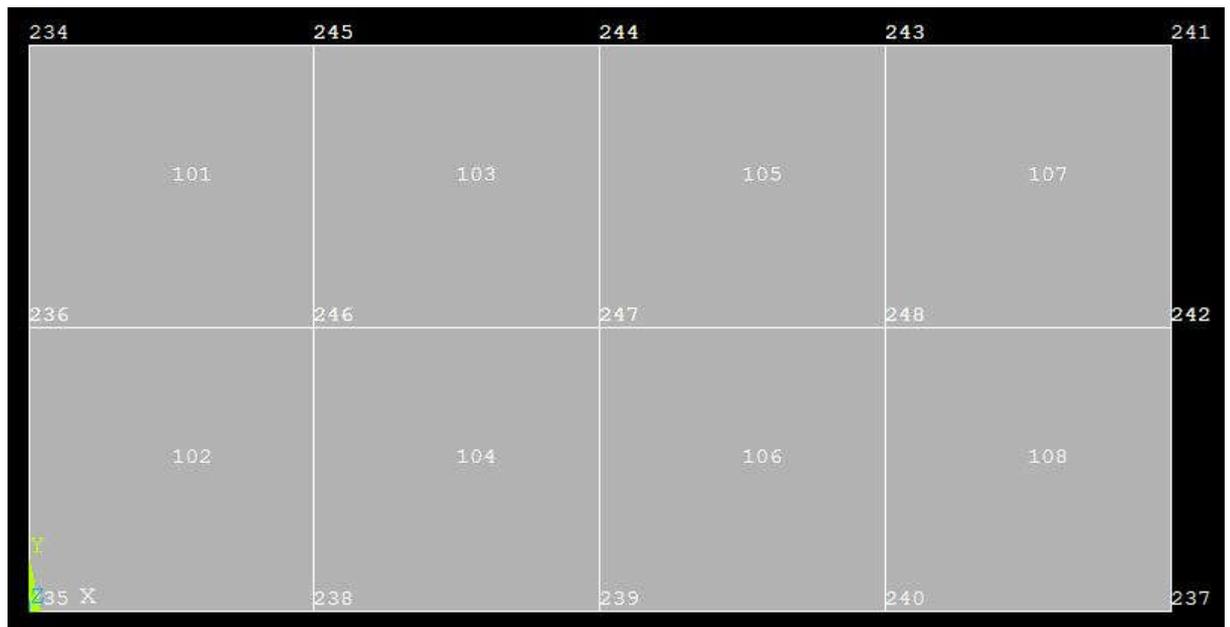Martensitic distribution after 10s is shown in figure 5.
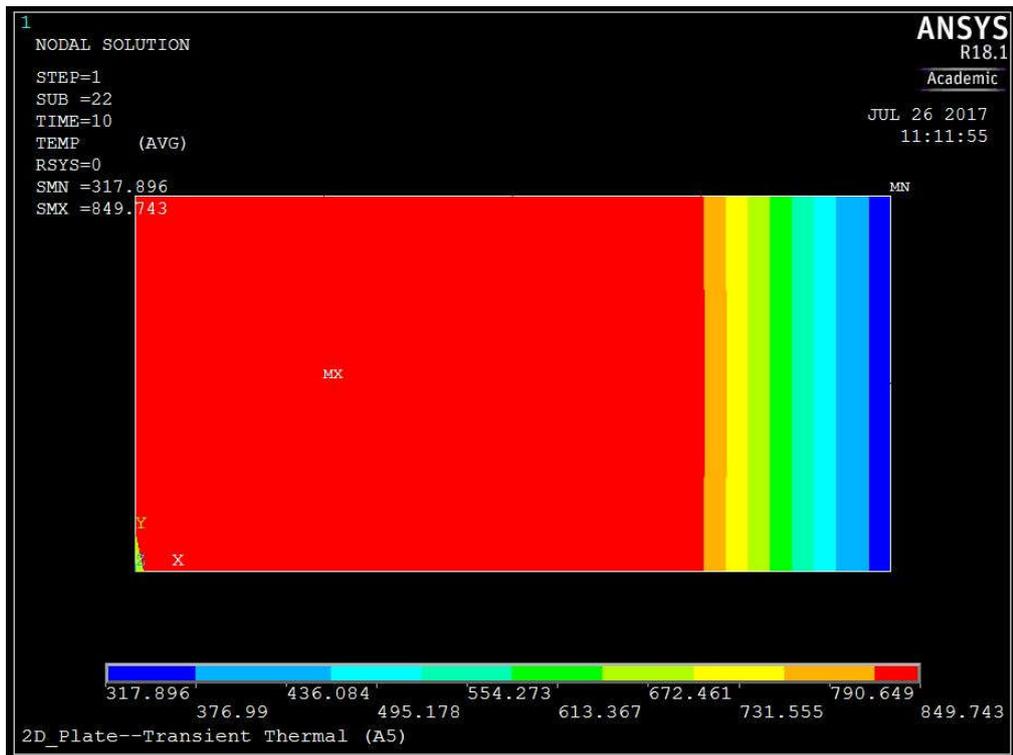

Figure 3. Geometry of 2D Plate

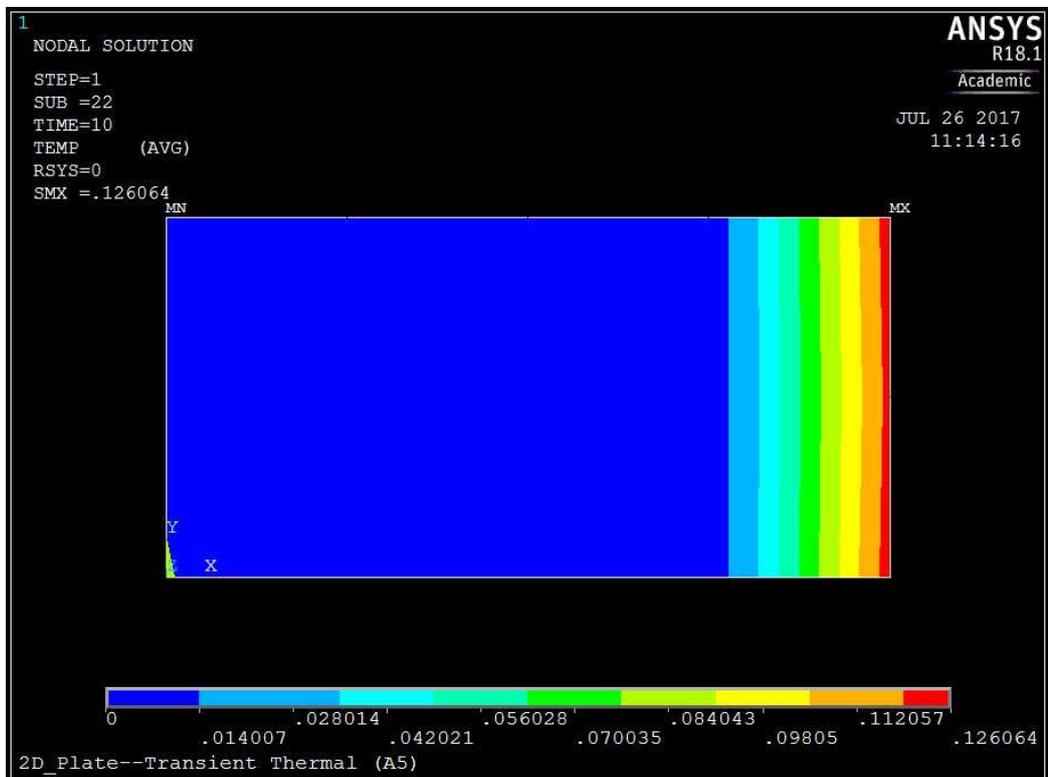Figure 4. Contour of Temperature distribution after 10s

Figure 5. Contour of Martensitic Fraction after 10s

Next, the same commands were little modified to run on workbench. The result of simulation is shown in figure 6. Corresponding Macros is as follows,

```
/POST1
SET,LAST
*GET, MAXND, NODE, ,NUM, MAX
*GET, MINND, NODE, ,NUM, MIN
NDS = MAXND - MINND + 1  !TOTAL NUMBER OF NODES

! DEFINE ARRAY: F(N) -- FRACTION OF PHASE TRANSFORMATION
*DIM, F, ARRAY, NDS,1

*SET,Ms,345 !From TTT diagram
*SET,Mf,130

    *DO, NN, 1, NDS
      *GET, TEM, NODE, NN+MINND-1,TEMP
      *IF, TEM, LE, Ms, THEN
              *IF, TEM, GE, Mf, THEN
                    F(NN) = (TEM-Ms)/(Mf-Ms)
              *ENDIF
       *ENDIF
    *ENDDO
/SHOW, PNG
*VPUT,F,NODE,MINND,TEMP
PLNSOL,TEMP
```
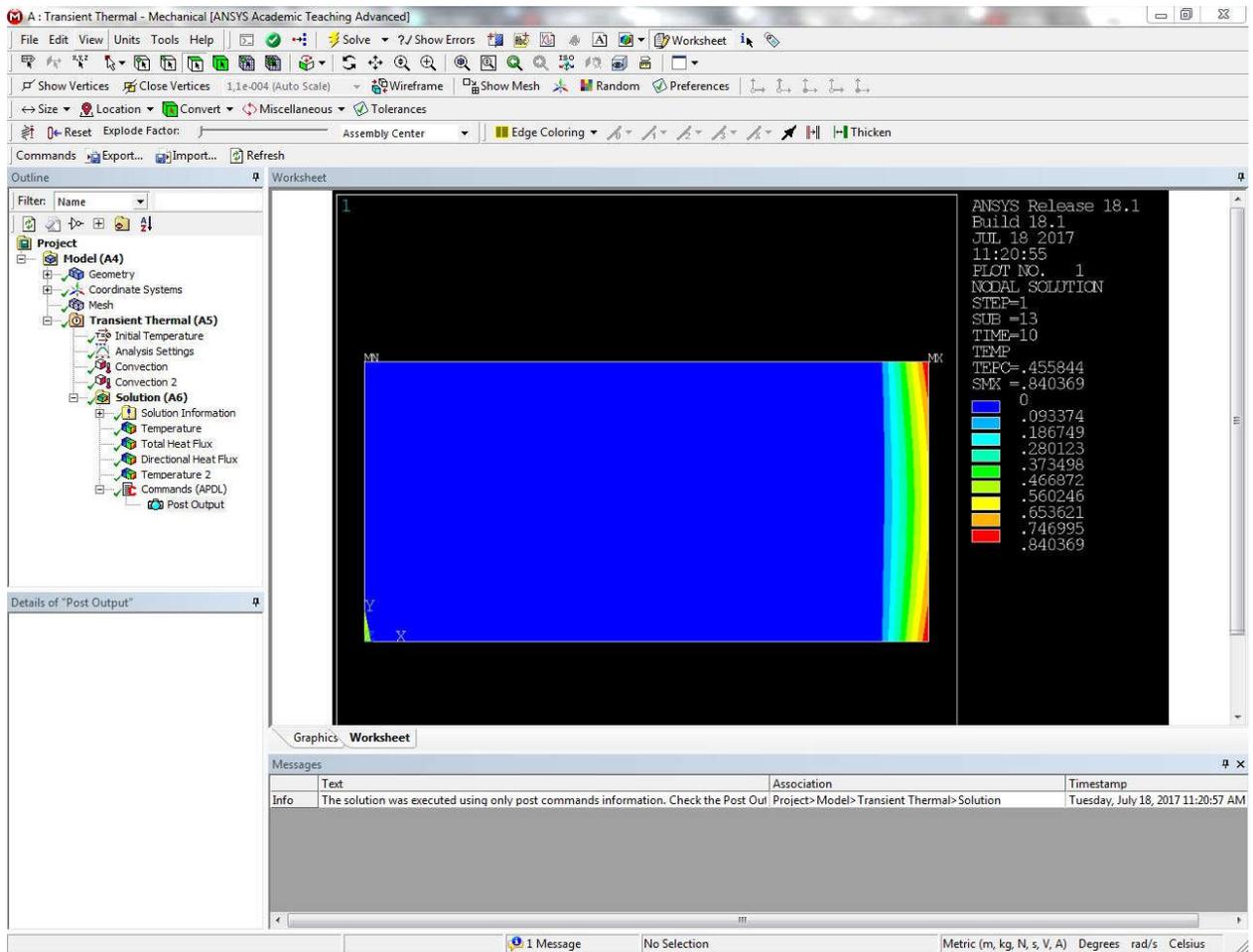
Figure 6. Contour of Martensitic Fraction after 10s from Workbench

To obtain more practical quenching simulation a 3D model is considered. A cylindrical component is considered with material 42CrMo4. The geometry with boundary conditions is shown in figure 7. Initially cylinder is at temperature 850°C which is above Austenitization temperature. Then transient thermal analysis is carried out in ANSYS Workbench. Figure 8 shows temperature distribution after 20 seconds. The lateral surface which is in contact with quenching water has lesser temperature and has more Martensitic fraction (Figure 9). And the core has least temperature and most martensitic content. This gives a rough idea of residual stresses due to microstructure. As Martensitic microstructure has more volume (less dense) compared to other grain structure, compressive stresses are induced in the component.
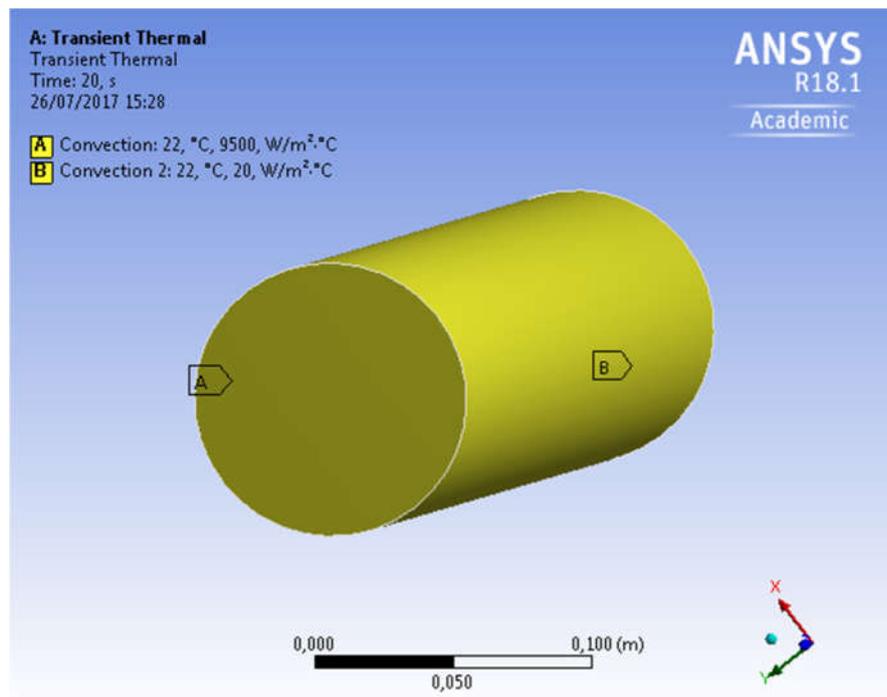
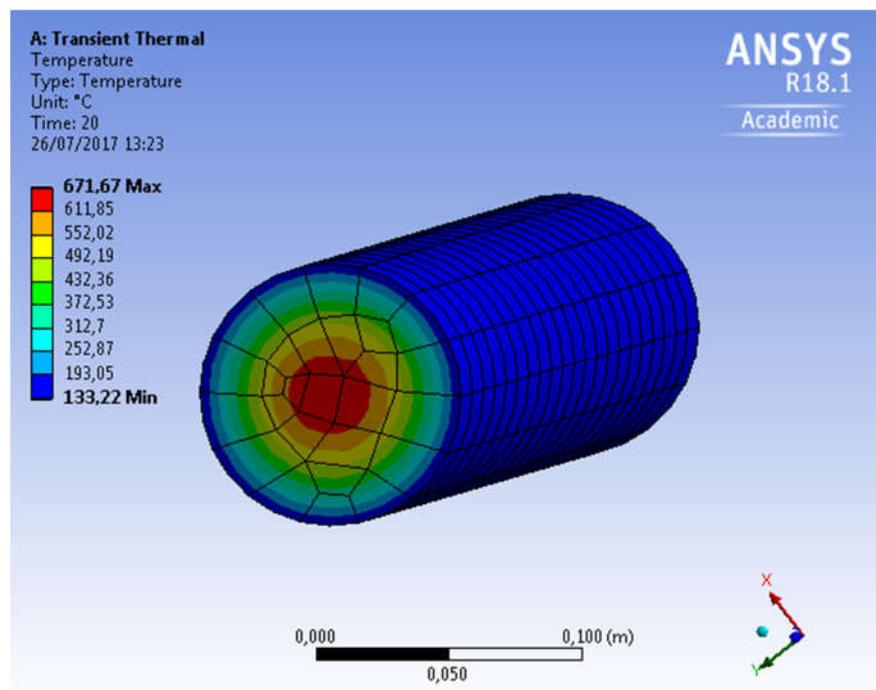Figure 7. Geometry of cylinder with Boundary conditions

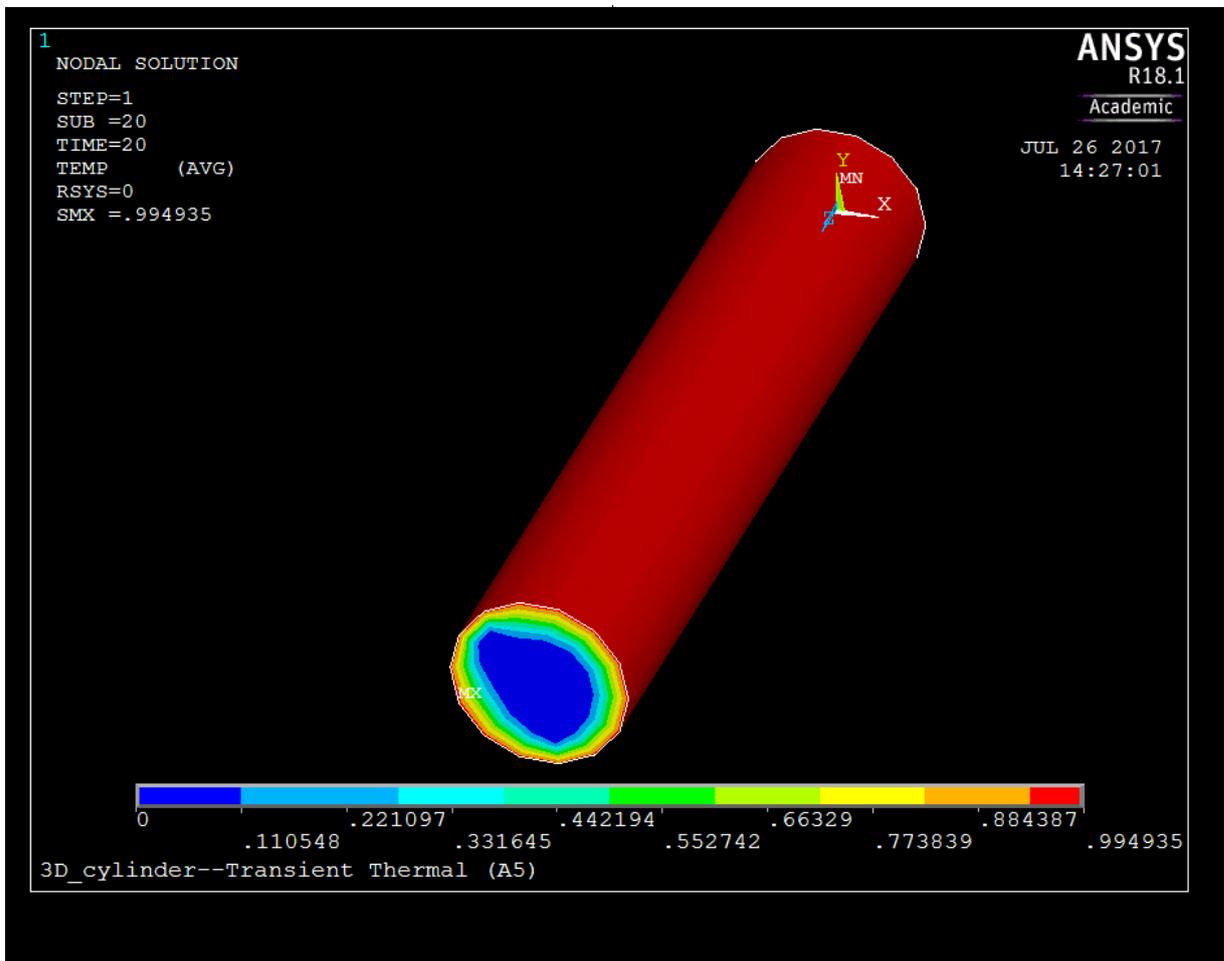Figure 8. Temperature contour diagram of Transient thermal analysis

Figure 9. Contour diagram of Martensitic fraction of cylindrical component

The simulation was compared with Koinstinen-Marbuger and results are shown in Figures 10 and 11. The Koinstinen-Marbuger equation is given by,

$$F(T_i) = F(T_i)_{max} \quad e^{-\gamma(M_s - T_i)}$$

Where, $\gamma = .011$ for most of the steels.

The magnitude of Martensitic fractions are lower in Koinstinen-Marbuger (exponential) model compared to linear model. Koinstinen-Marbuger equation is better suitable for continuous cooling (CCT) model. Macro for Koinstinen-Marbuger equation is as follows,

```
/POST1
SET,LAST
*GET, MAXND, NODE, ,NUM, MAX
*GET, MINND, NODE, ,NUM, MIN
NDS = MAXND - MINND + 1  !TOTAL NUMBER OF NODES

! DEFINE ARRAY: F(N) -- FRACTION OF PHASE TRANSFORMATION
*DIM, F, ARRAY, NDS,1

*SET,Ms,345 !From TTT diagram
*SET,Mf,130

    *DO, NN, 1, NDS
      *GET, TEM, NODE, NN+MINND-1,TEMP
      *IF, TEM, LE, Ms, THEN
              *IF, TEM, GE, Mf, THEN
                    F(NN) = 1-exp(-0.011*(Ms-TEM))
              *ENDIF
       *ENDIF
     *ENDDO
/SHOW, PNG
*VPUT,F,NODE,MINND,TEMP
PLNSOL,TEMP
```
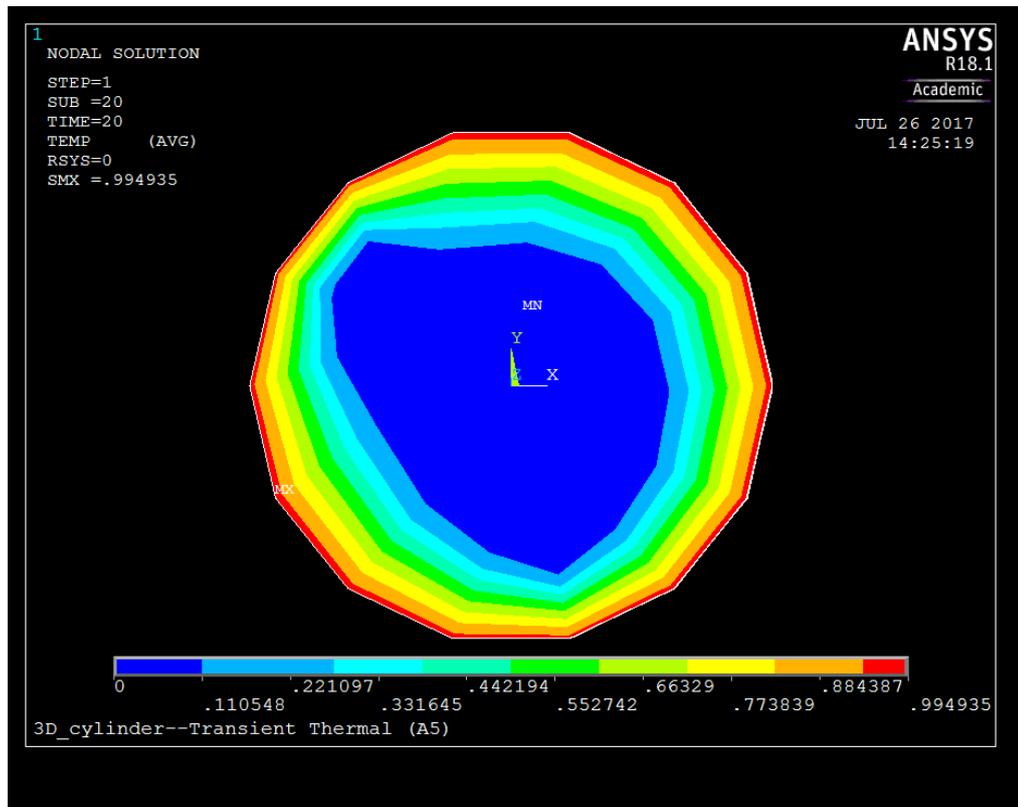
Fig 10. Martensitic fraction using linear relation with temperature
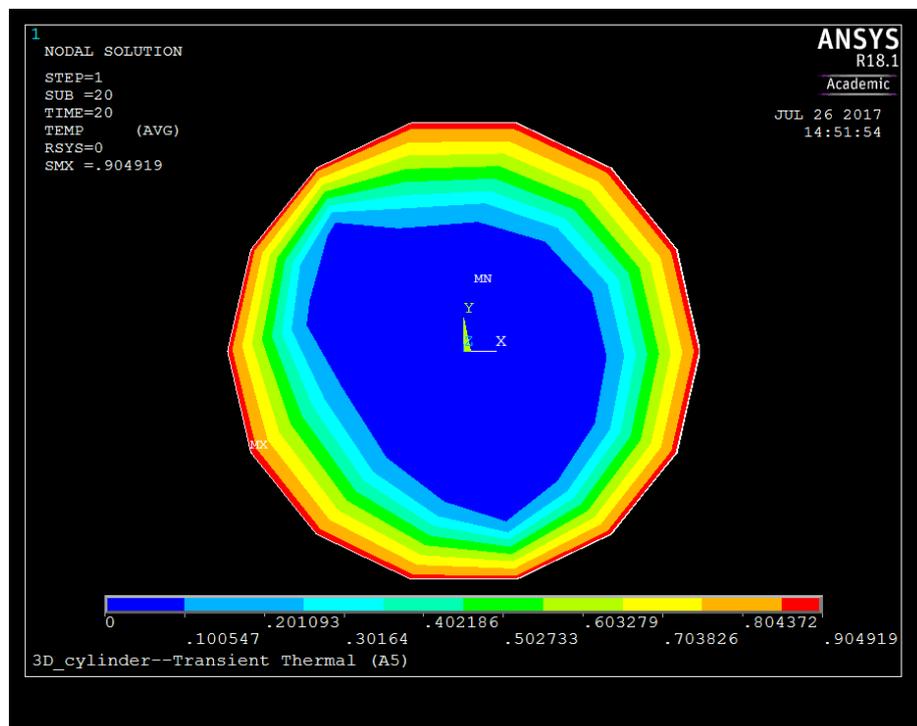

Fig 11. Martensitic fraction using Koinstibnen-Marbuger Equation

It's always advisable to simply algorithm before simulation. To decide whether to consider Bainite, Perlite and Ferrite for quenching simulation following cooling curves are plotted. For the same cylindrical component, four nodes are considered to plot cooling curves; one at the center, one at the surface and remaining two in between (refer Figure 12). One at the center is most crucial to decide. Figures 13 to 16 shows cooling curves at time 10s, 20s, 60s and 100s respectively. From the plots it is clear that quenching does not include Pearlite and Ferrite microstructure. But, a small portion do fall under Bainite region in CCT or TTT diagrams. Hence, Bainite microstructure to be considered for more practical results.
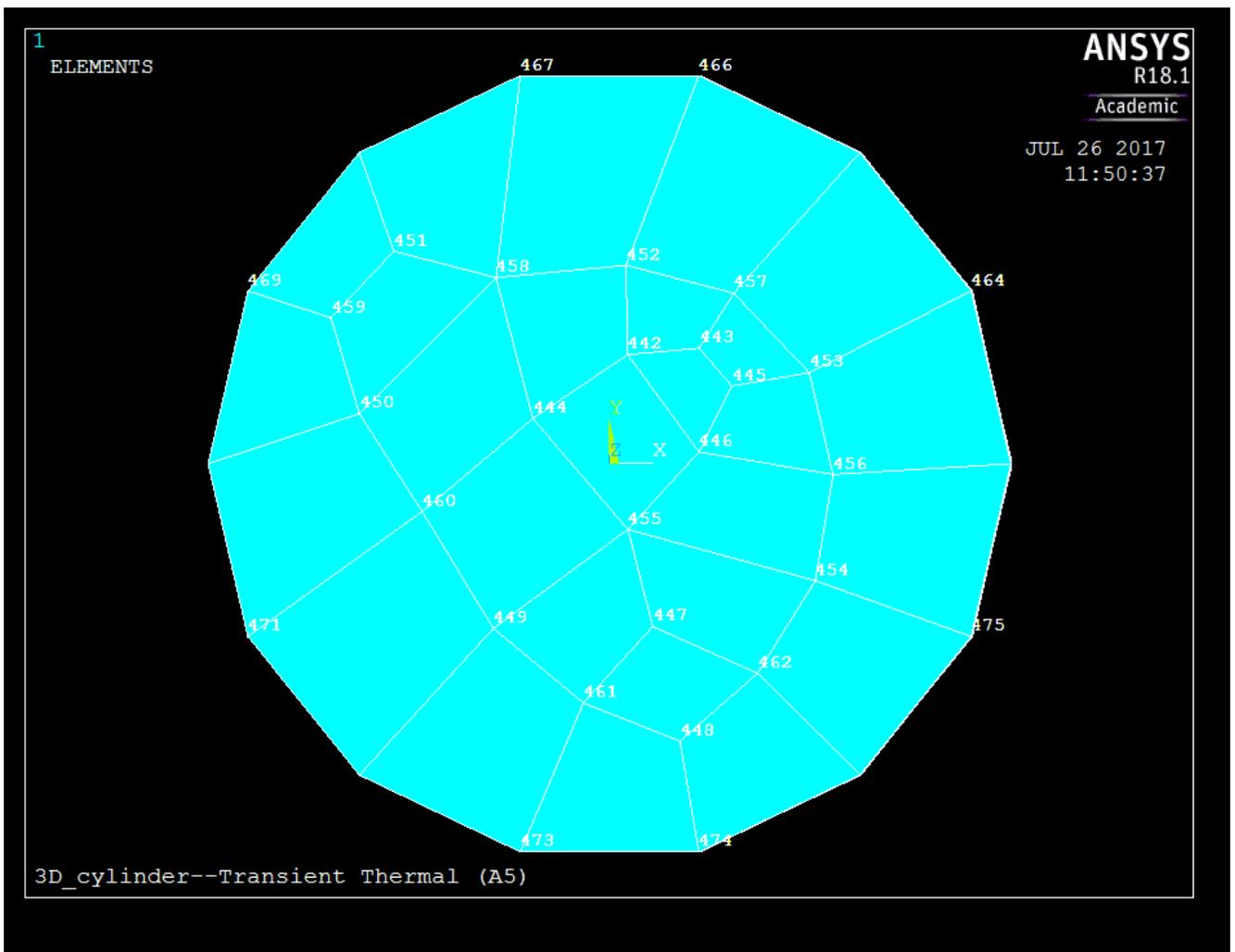

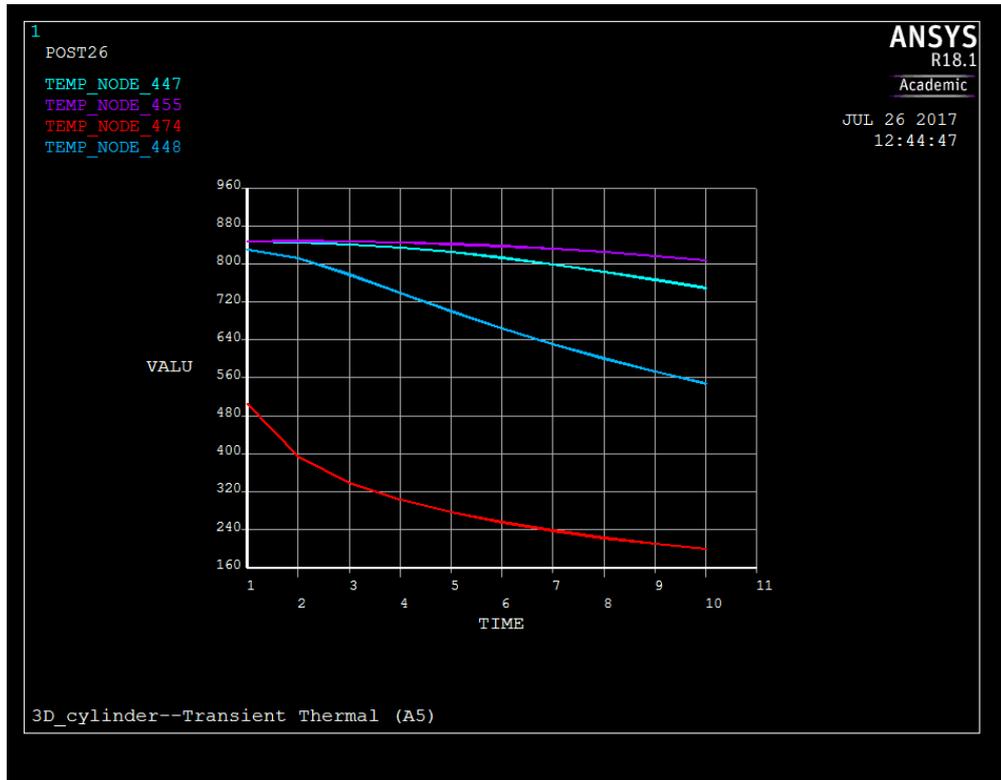Figure 12. Geometry of cylinder with node numbers
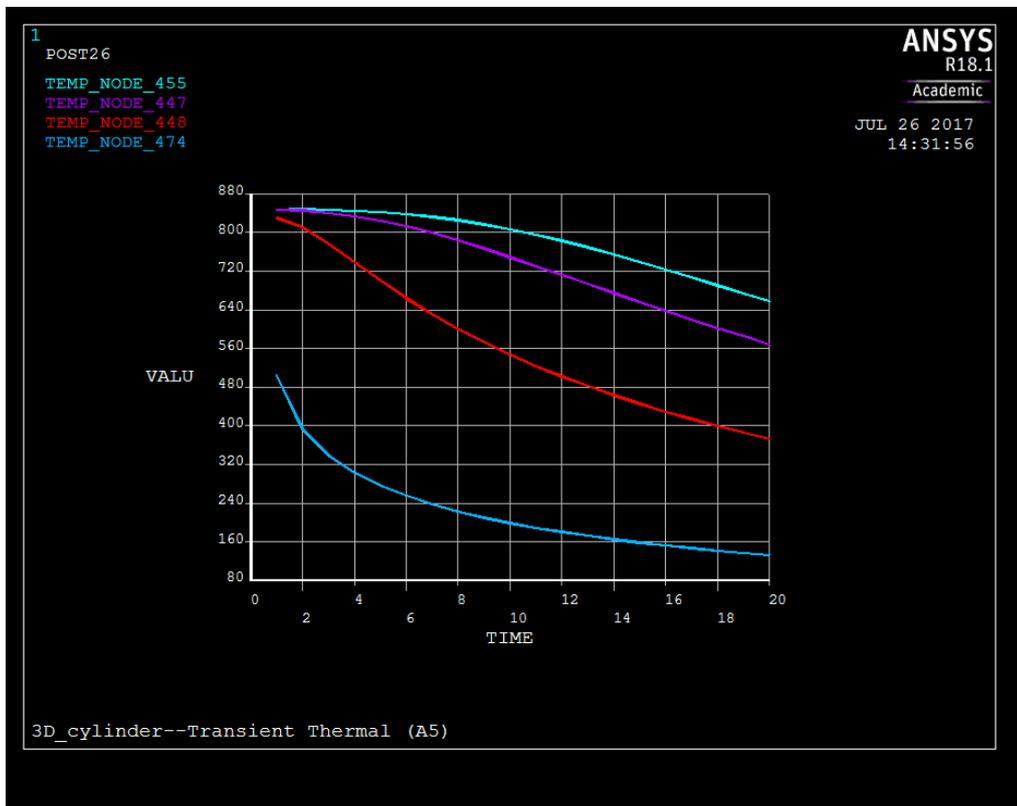
Figure 13. Cooling curves after 10s
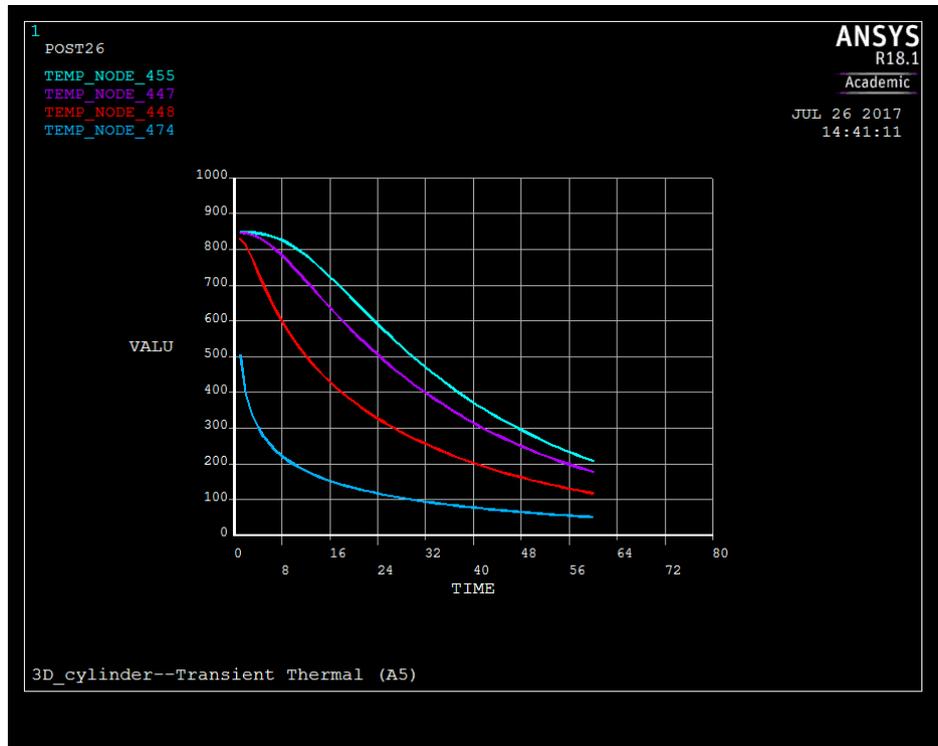

Figure 14. Cooling curves after 20s

Figure 15. Cooling curves after 60s
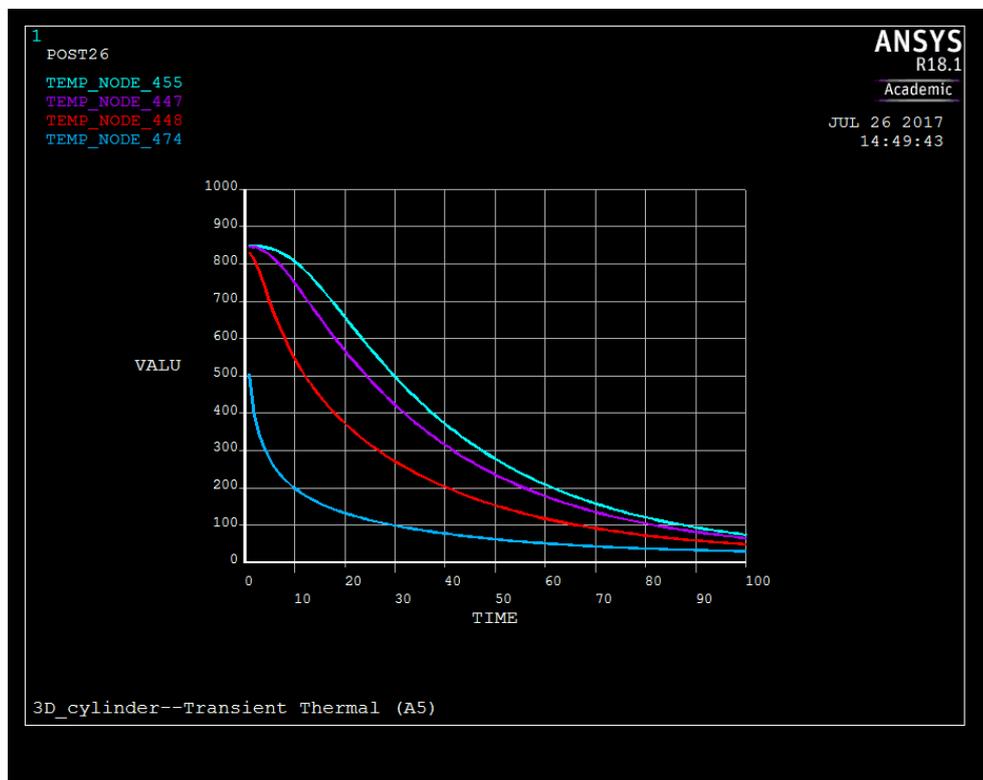
Figure 16. Cooling curves after 100s

Figure 17 summarizes the cooling rates with CCT diagram. Ferrite and Pearlite can be completely ignored, as quenching is a fast cooling process.
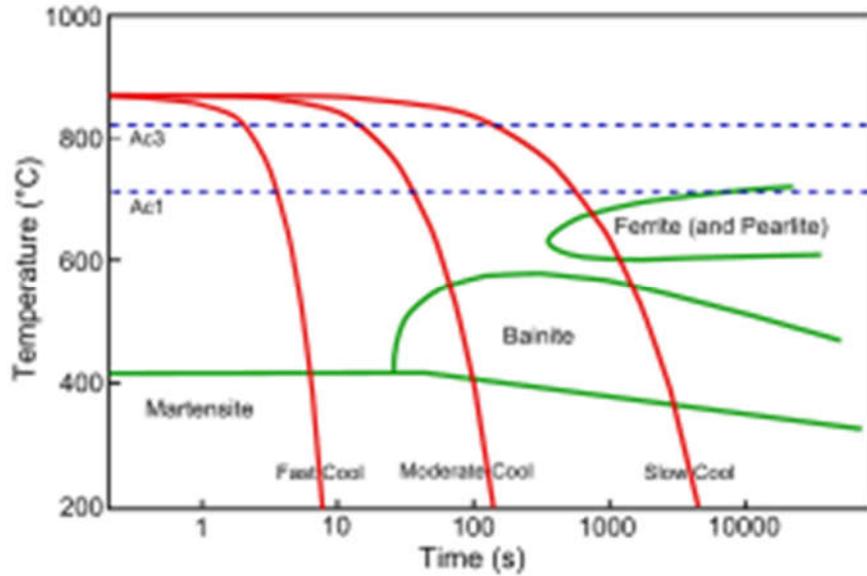
Figure 17. Cooling curves with CCT

A sample code based on Avrami (JMAK) Equation is available from reference 2. It's based on Isothermal model, hence, thermal history input was fed from TTT diagram of steel 42CrMo4. Corresponding TTT diagram is shown in Figure 18 (ref. 8). For a specific set of temperatures, transformation start and end times are noted and they are stored as arrays.
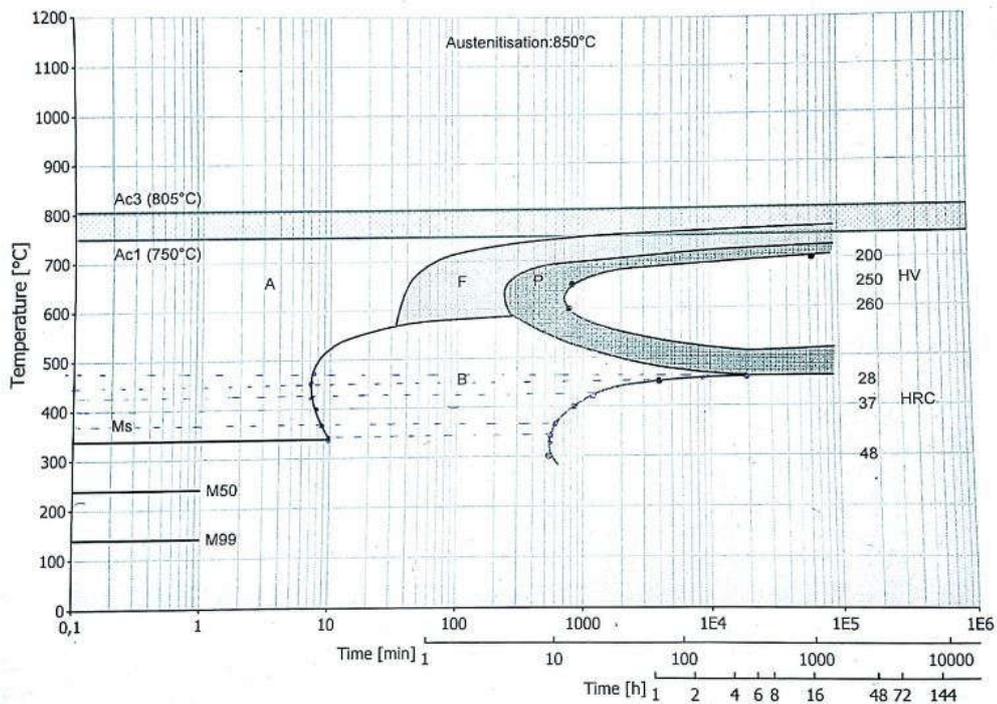
Figure 18. TTT diagram of Steel 42CrMo4

Sample code to implement Avrami (JMAK) equation is as follows,

```
/POST1
*GET, MAXND, NODE, ,NUM, MAX
*GET, MINND, NODE, ,NUM, MIN
NDS = MAXND - MINND + 1
! DEFINE ARRAY: F(N) -- FRACTION OF PHASE TRANSFORMATION
*DIM, F, ARRAY, NDS
! DEFINE ARRAY: ET () -- INCUBATION
*DIM, ET, ARRAY, NDS
!ARRAYS TO STORE TTT DIAGRAM
*DIM, TNM, ARRAY, 6, 1
TNM(1)= 475, 450, 430, 400, 365, 345
*DIM, TH1, ARRAY, 6, 1
TH1(1)= 7.5, 7, 7.25, 8, 9, 10
*DIM, TH2, ARRAY, 6, 1
TH2(1) = 20000, 4000, 1300, 850, 600, 550

*SET,DT,1
*SET,TS,345
*SET,F(1,1),0
*SET,ET(1,1),0

*DO, NN, 1, NDS
        !QT = 0
        !BF, NN+MIIND-1, HGEN, 0
        *IF, F(NN), LE, 0.95, THEN
                *GET, TEM, NODE, NN+MIIND-1, TEMP
                *DO, K, 1, 5, 1
                        *IF, TEM, LE, TNM(K), THEN
                                *IF TEM, GE, TNM(K+1), THEN
                                        TIME1 = TH1(K)-(TH1(K)-TH1(K+1))*(TNM(K)-
TEM)/(TNM(K)-TNM(K+1))
                                        TIME2 = TH2(K)-(TH2(K)-TH2(K+1))*(TNM(K)-
TEM)/(TNM(K)-TNM(K+1))
                                *ENDIF
                        *ENDIF
                *ENDDO
                *IF, TEM, GT, TNM(1), THEN
                        TIME1 = TH1(1)
                        TIME2 = TH2(1)
                *ENDIF
                *IF, TEM, LT, TNM(6), THEN
                        TIME1 = TH1(6)
                        TIME2 = TH2(6)
                *ENDIF
```

```
TN = LOG(LOG(0.95)/LOG(0.05))/LOG(TIME1/TIME2)
TK = -LOG(0.95)*10000.0/TIME1**TN
TT = TIME1
*IF, TEM, LE, TS, THEN
        TT = 1.0E10
*ENDIF
ET(NN) = DT/TT+ET(NN)
*IF, ET(NN), GT, 0.98, THEN
        TJ = (-LOG(0.99-F(NN))*10000.0/TK)**(1.0/TN)
        TJJ = -TK*(TJ+DT)**TN/10000.0
        *IF, TJJ, LE, -50, THEN
                TJJ = -50;      ! AVOID UNDERFLOW OF EXP FUNCTION
        *ENDIF
        !FT = 1.0 - EXP(TJJ) - F(NN)
        !QT =  -DH*FT/DT
        ! INPUT AS HEAT GENERATION RATE:
        !BF, NN+MIND-1, HGEN, QT
        F(NN) = 1.0 - EXP(TJJ)
    *ENDIF
  *ENDIF
*ENDDO

/SHOW, PNG
*VPUT,F,NODE,MINND,TEMP
PLNSOL, TEMP
```

This code was tested for the cylindrical component, but it was not successful to give necessary results. The code is valid only for Isothermal processes. For quenching (non-isothermal) this code is to be modified to apply Avrami equations over small time intervals [1]. Alternative option is to develop an algorithm based on CCT diagrams.

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5. CONCLUSIONS AND FUTURE SCOOPE

Using available software packages, in IKERLAN there are two possible options are for Induction hardening.

1) Electromagnetic simulation in FLUX and quenching simulation in Code Aster.

2) Electromagnetic, Thermal, Mechanical simulation in ANSYS Workbench and Microstructure simulation using APDL macros.

Initially second option seemed to be a better one. Macros were developed for Martensitic transformation and microstructure simulation was successful for fast cooling processes. As Martensitic transformation depends only on temperature the results were satisfactory. Extending it to moderate cooling to consider Bainite region and also to include latent heat of transformation is tedious job. This could be possible by applying isothermal algorithm over small time interval [1]. But, using CCT diagrams for simulation will be more practical. Developing algorithm to use CCT for microstructure simulation is an interesting and challenging task ahead.

First option would be a good alternative for induction hardening; as in Code Aster most of the code words and documents are freely available. If the codes are fully developed for Non isothermal model, it would be worth considering to work on Code Aster.

6.   REFERENCES

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