A Practical and Integrated Approach to Heat Treatment Simulation of Steel

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Virtual Faculty Development Program on
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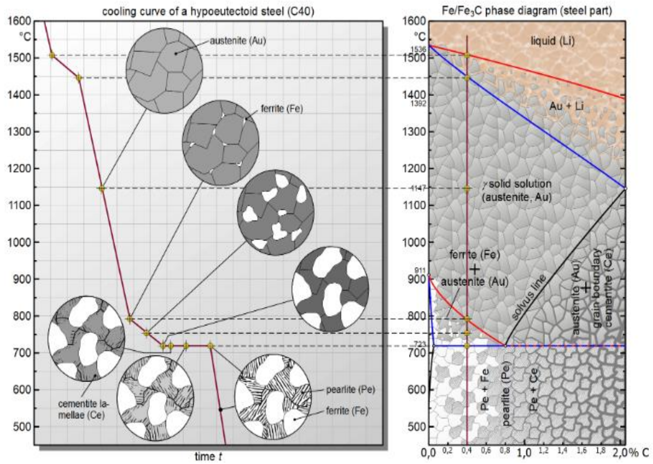
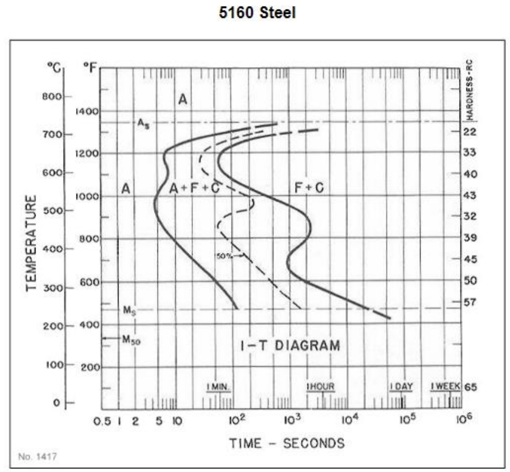
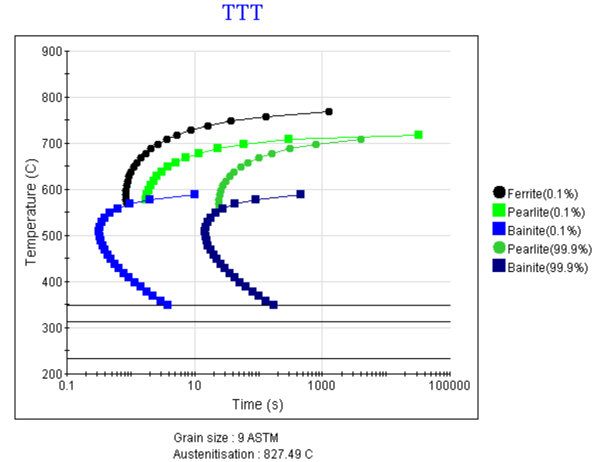
Challenges in Quench Heat Treatment Simulation

- Modeling preheating in furnaces
  - Not something to be ignored – potential for energy saving
- Effect of Transfer Time from Furnace to Quench Tank (large components)
  - Minimum temperature above Ae3 must be ensured, edges cool faster than surfaces
- Modeling Microstructure Evolution during Quenching
  - Compromise between equilibrium and TTT diagrams
- Heat Transfer during Quenching
  - Two phase heat transfer, not properly quantifiable; all three phases present simultaneously – film boiling, nucleate boiling and convective heat transfer
- Development of Proper Tools for Measuring HTC / Heat Flux Rate during Quenching
  - Measurement of HTC in plant conditions, a major challenge (Equipment design and Estimation)
- Modeling Hardness of as-Quenched Structures
  - Varies with composition and quenching rates – a property defined by the process route, not just by the composition!
- Stresses, Cracks and Distortion
  - Material characterization at high temperatures – Elastic / Plastic / Viscoelastic ?
- Modeling Tempered Hardness
  - Effect of both time and temperature

Understanding Metallurgy of Steels







The Fe-C equilibrium diagram is not of much use to Modeling Heat Treatment

- The Fe-C (Fe-Fe3C) diagram is an equilibrium diagram
- Steel is a multicomponent alloy
- The equilibrium Diagram is a Binary Diagram
- The effect of other alloying elements are considered through defining a Carbon Equivalent
- There are many formulae for CE

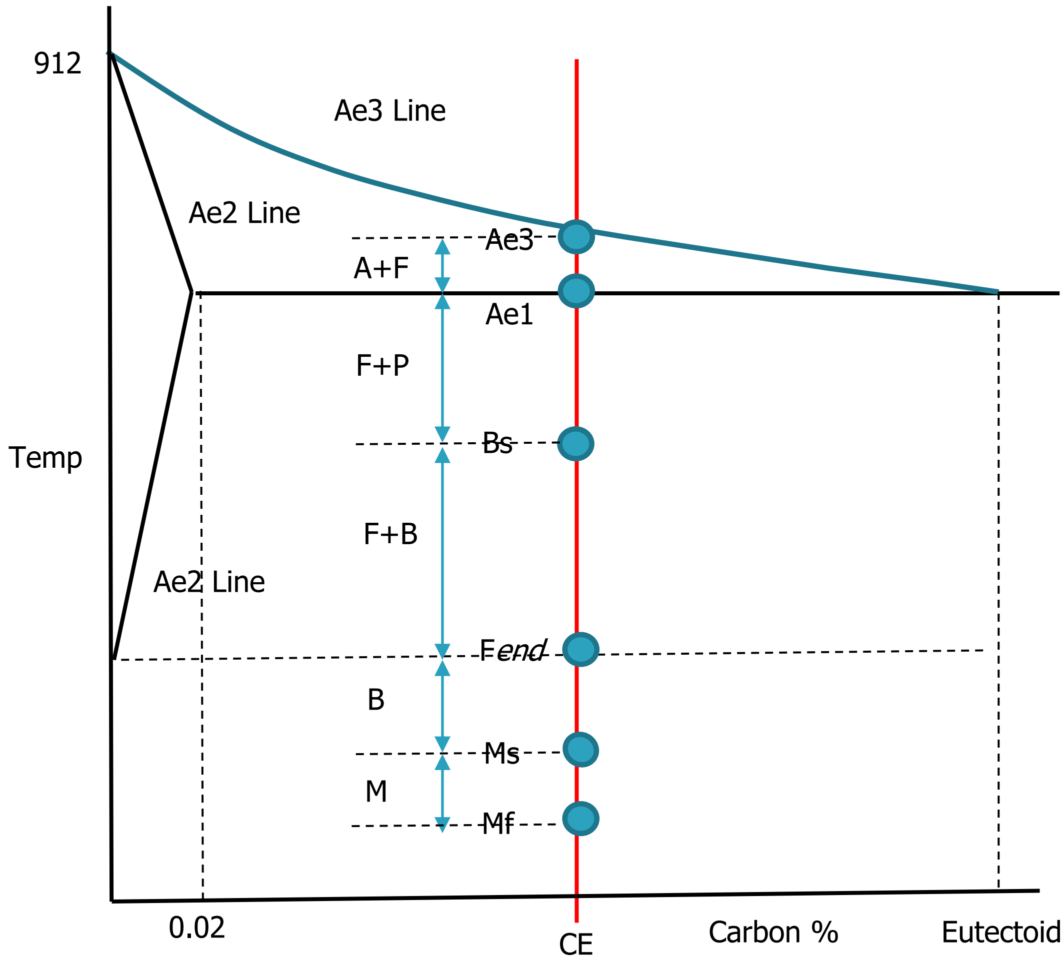
The TTT diagram provides basic information for modeling Heat Treatment

- Shows non-equilibrium phases
- Isothermal transformation which is practically impossible
- The effect of all alloying elements are considered
- Experimentally obtained – Grade Specific (Atlas of TTT)

Calculated TTT diagram from first principles – Composition Specific (JMatPro)

- **Neither Fe-C Equilibrium Diagram nor the TTT diagram can be independently used for heat treatment simulation for both have deficiencies**
- **We need to use the information from both diagrams and develop an appropriate diagram for tracking austenite decomposition**

Critical Temperatures – Importing TTT Data onto Fe-C Equilibrium Diagram



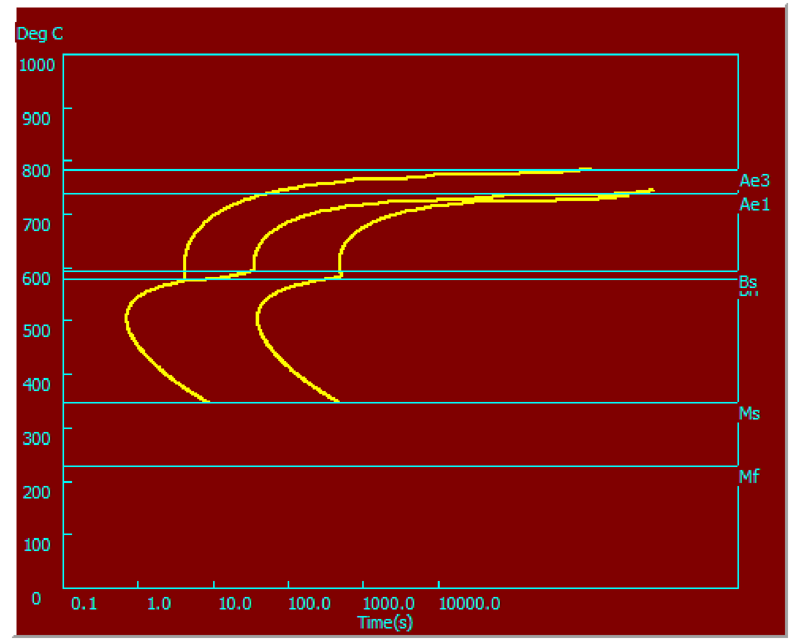
Ae_3 boundary was obtained by a standard regression equation

Ae_3=912-203$C^{0.5}$+15.2Ni+44.7Si-104V+31.5Mo+13.1W-30Mn-11Cr-20Cu+700P+400Al+120As+ 400Ti

Ae_1 temperature for the steel was read off from the TTT diagram for the steel grade

Ae_3 temperature for the steel was read off from the TTT diagram for the steel grade, fixing CE

Bs, F*end*, Ms *and* M*f* were obtained by TTT Diagram



Austenite Transformation Models

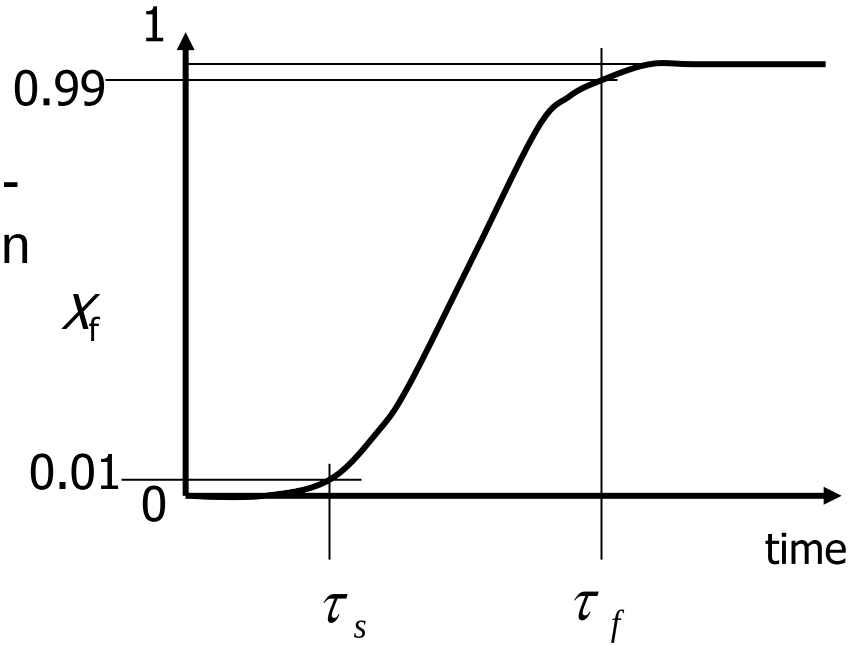
Austenite – Ferrite/Pearlite/Bainite:

Diffusion controlled JMAK (Johnson-Mehl-Avrami-Kolmogoroav) Equation

$$X_i^{\,j} = 1 - \exp[-b(T_j)\; t_j^{\,n(T_j)}]$$

$$n(T_j) = \frac{\ln[\ln(1 - X_s)/\ln(1 - X_f)]}{\ln(\tau_s/\tau_f)}$$

$$b(T_j) = -\frac{\ln(1 - X_s)}{t_s^{\,n}}$$

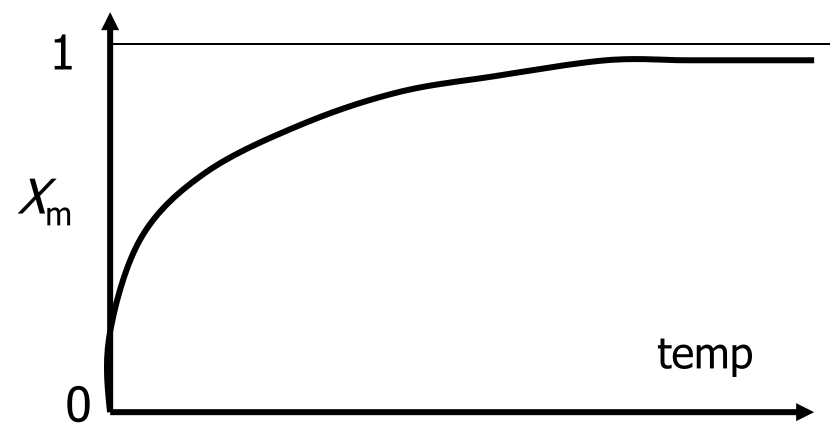


Austenite – Martensite:

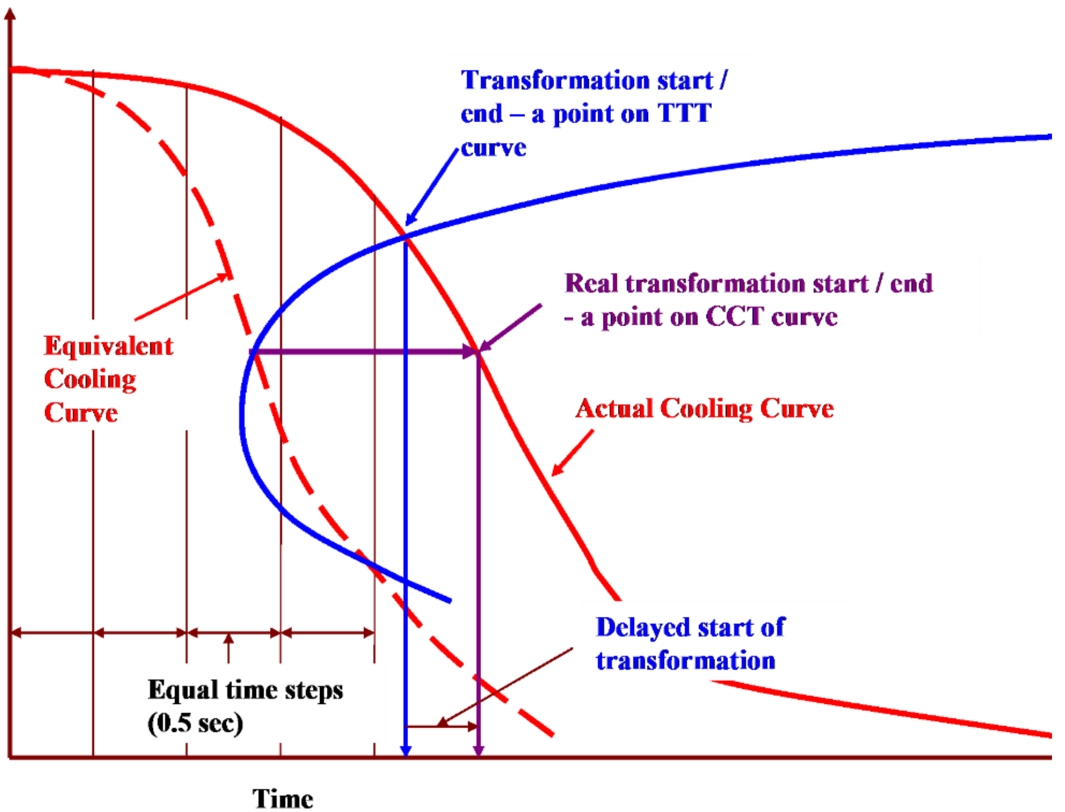
Diffusion less KM (Koistenin-Marburger) Equation

$$X_m = 1 - \exp[-\Omega(M_s - T)]$$

Ω obtained by the X_m value at M_f



Generating CCT Diagrams from TTT Diagrams



Scheil's additivity rule for marking transformation begin:

$$\sum_{j=1}^{m} \frac{\Delta t_j}{t_s(T_j)} \geq 1$$

Real fraction transformed:

$$X^i_{norm}(T_m) = \frac{X^i_{real}(T_{m-1})}{X^i_{eqbrm}(T_m)}$$

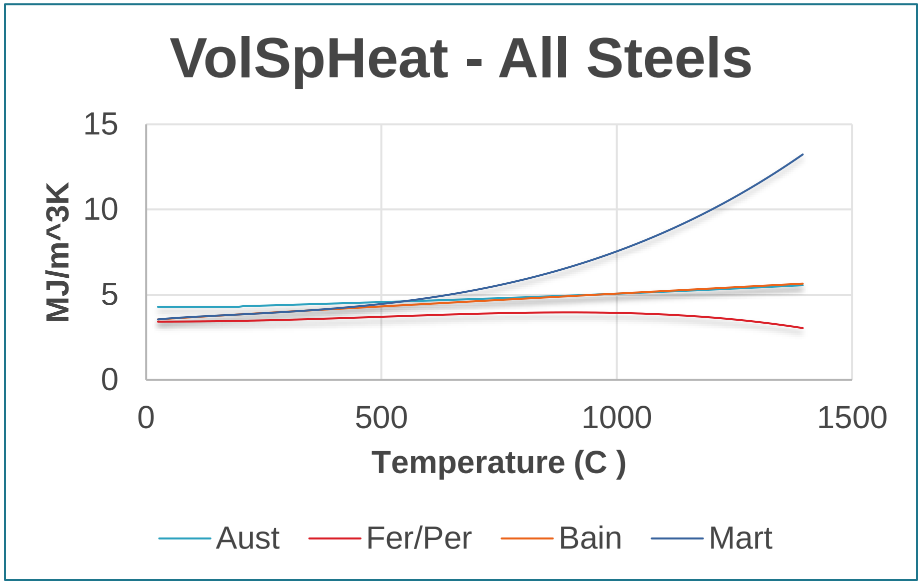
$$t^i_{eq} = \left[\frac{-\ln\left[1 - X^i_{norm}(T_m)\right]}{b(T_{m+1})}\right]^{\frac{1}{n(T_{m+1})}}$$

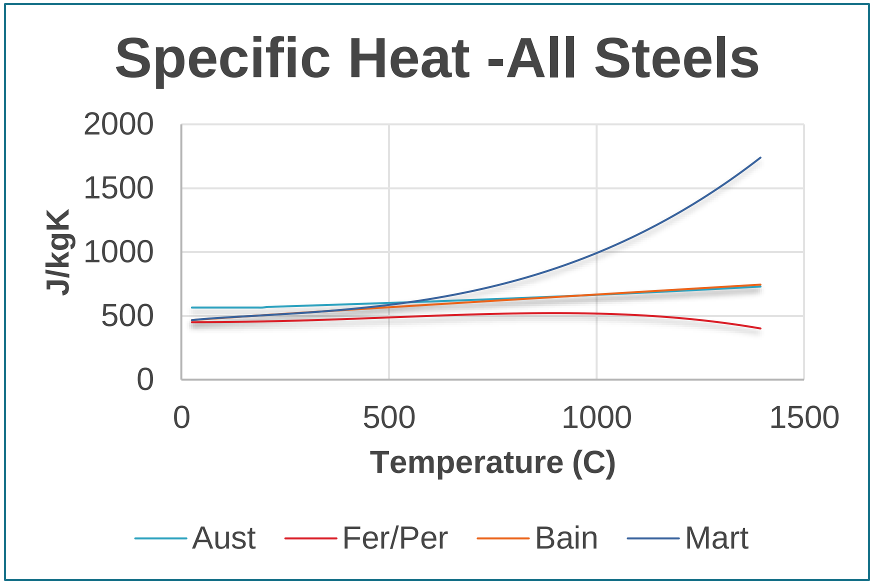
$$X^i_{norm}(T_{m+1}) = 1 - \exp[-b(T_{m+1})\left(t^i_{eq} + \Delta t\right)^{n(T_{m+1})}]$$

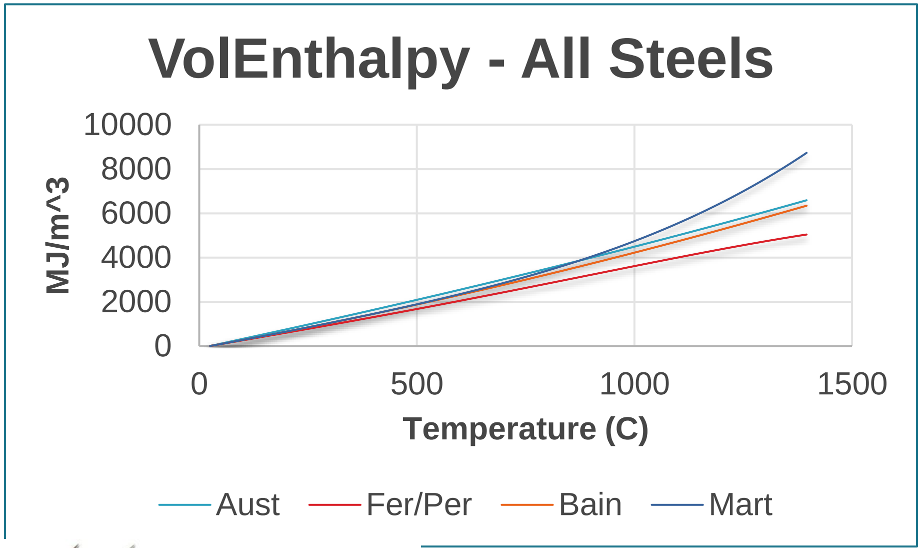
$$X^i_{real}(T_{m+1}) = X^i_{norm}(T_{m+1}) X^i_{eqbrm}(T_{m+1})$$

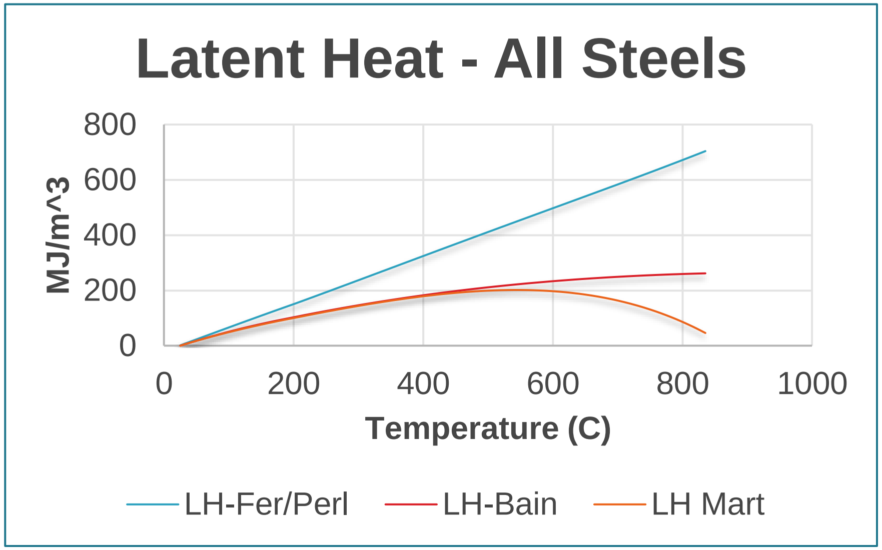
Obtaining the CCT curve using TTT curve and calculated temperature

Steel Properties – Common to all Grades





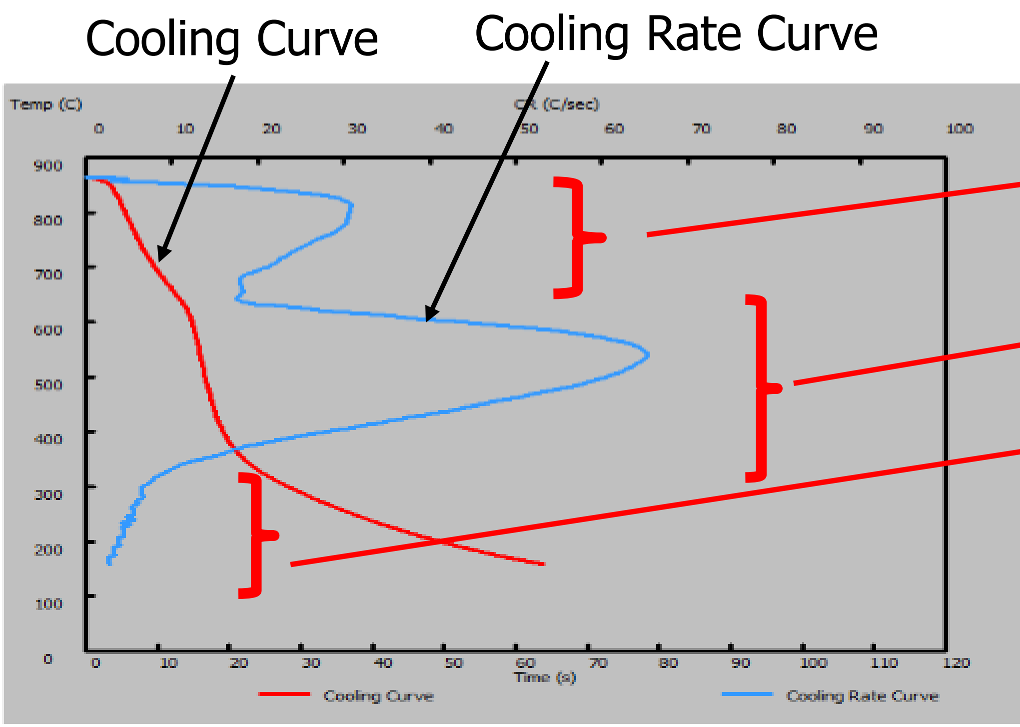


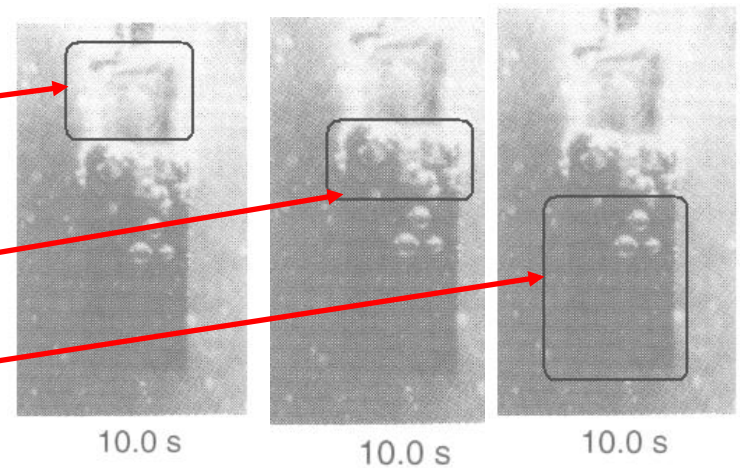


Input on Steels – A Summary

- Correct interpretation of critical information (Ac3, Ae1, Acm, CE etc.)
- Reconciliation of Equilibrium and TTT data on steels
- Composition specific TTT diagram (if not at least grade specific)
- Distinct regimes of ferrite, pearlite, bainite and martensite transformation especially in the case of high alloy steels
- An algorithm to track austenite transformation as the steel cools – generate CCT curves
- Thermophysical properties of different phases

Heat Transfer during Quenching





Film boiling phase: Heat transfer impeded by a vapor blanket

Nucleate boiling phase: Maximum heat transfer due to wetting

Convective Phase: Low heat transfer through convection

- **For simulating quenching, we must know the HTC (Heat Transfer Coefficient) during quenching**.
- Boiling heat transfer is one of the most complex heat transfer phenomenon to quantify.
- A special tool – 'Reference Quench Probe' has been developed to measure HTC during quenching in various quenchants

"Handbook of Quenchants and Quenching Technology," 1993, Eds: G.E.Totten, C.E.Bates, N.A.Clinton, ASM

Measurement of HTC During Quenching

A new tool 'Reference Quench Probe' has been designed for measuring boiling heat transfer

Designed for portability and *in-situ* testing

The specimen has been redesigned for testing different section sizes

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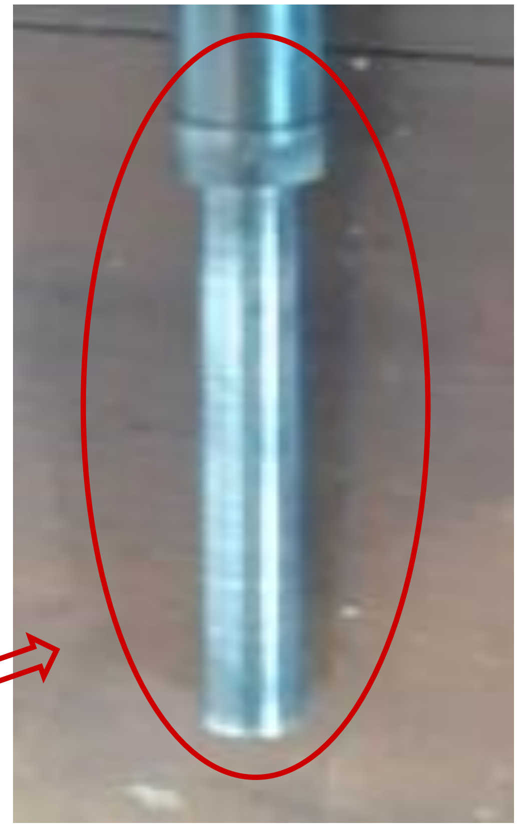
Quench specimen for HTC determination as function of section thickness

Setup for estimating Heat Transfer Coefficient during Quenching in Laboratory Condition

Temperature recorder

Furnace

Probe



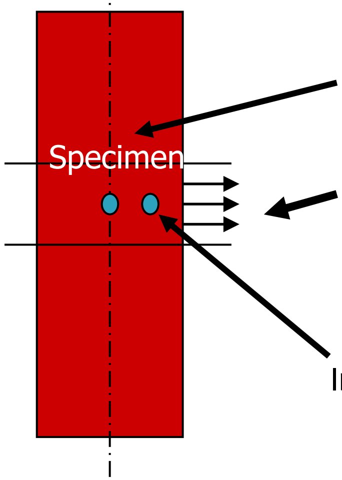
Steel Sample

Quench Vessel

Theory of Reference Quench Probe – Inverse Heat Transfer*

- Boiling heat transfer cannot be easily measured or calculated using CFD
- Since the temperature can be easily measured, we use the temperature data as input and calculate the heat flux rate
- This is known as the INVERSE Heat Transfer Problem, a very difficult problem to solve, developed* in 2004.

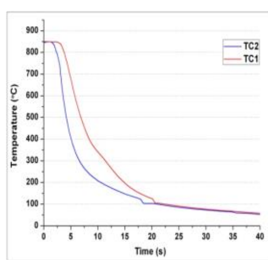
$$k\frac{\partial}{\partial r}\left(\frac{\partial T(r,z,t)}{\partial r}\right)+k\frac{\partial}{\partial z}\left(\frac{\partial T(r,z,t)}{\partial z}\right)+\dot{q}=\rho c\frac{\partial T(r,z,t)}{\partial t}$$

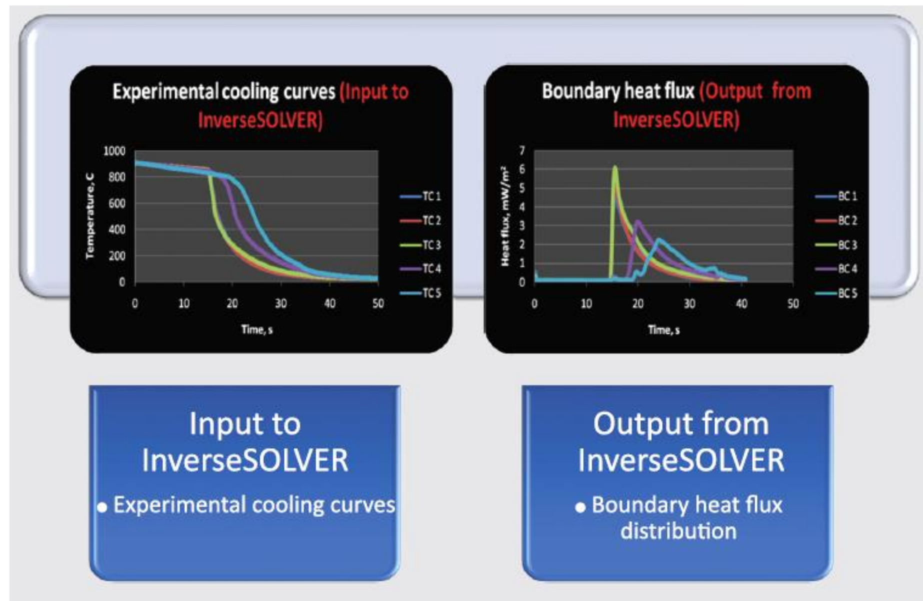


IC: $T(r,z)=T_{soaking}$

BC: $-k\left(\frac{\partial T}{\partial r}n_r\right)=q=?$ — To be solved

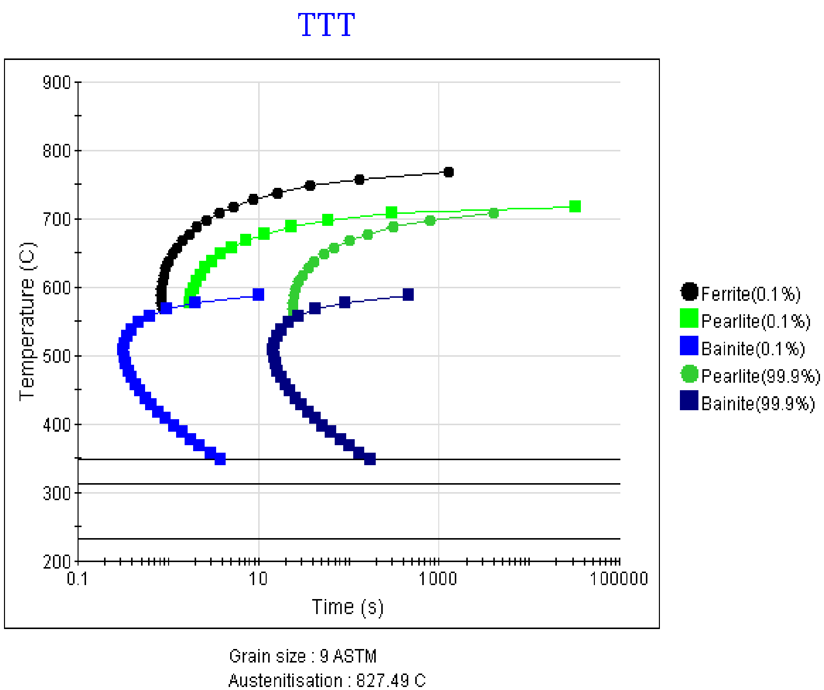
Input:





*T.S.Prasanna Kumar "A serial solution for the 2-D inverse heat conduction problem for estimating multiple heat flux components"- Numerical Heat Transfer Part B-Fundamentals, Vol 45, n 6, June, 2004, pp 541-563

Theory of Reference Quench Probe – Metallurgical Model



Calculated TTT diagram from first principles – Composition Specific (JMatPro)

Austenite – Ferrite/Pearlite/Bainite

$$X_i^{\,j} = 1 - \exp[-b(T_j)\, t_j^{\,n(T_j)}]$$

$$n(T_j) = \frac{\ln[\ln(1 - X_s)/\ln(1 - X_f)]}{\ln(\tau_s / \tau_f)}$$

$$b(T_j) = -\frac{\ln(1 - X_s)}{t_s^{\,n}}$$

Austenite - Martensite

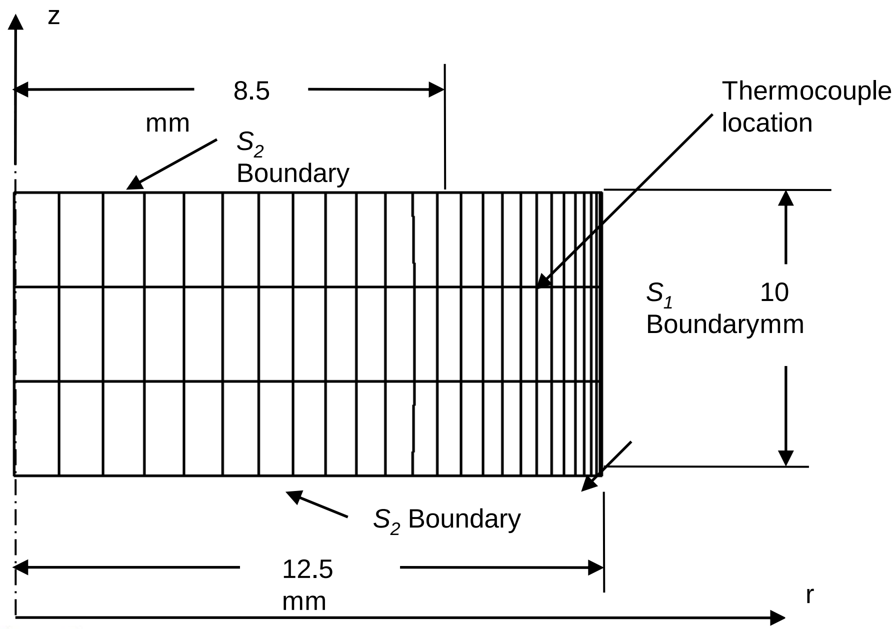
$$X_m = 1 - \exp[-0.011(M_s - T)]$$

Theory of Reference Quench Probe – Finite Element Analysis

Iterative FE formulation within time step for non linear problems:

$$\left(\Delta t\theta[K]_{n+1}^{l+1}+[C]_n\right)\{T\}_{n+1}=\left([C]_n-\Delta t(1-\theta)[K]_n\right)\{T\}_n+\Delta t(1-\theta)\{F\}_n+\Delta t\theta\{F\}_{n+1}^{l+1}$$

$$C_{ij}=\int_{\Omega^e}\left[\rho c-\rho\Delta H\left(\frac{\Delta f}{\Delta T}\right)\right]\psi_i\psi_j\,d\Omega \qquad K_{ij}=\int_{\Omega^e}\left[k\frac{\partial\psi_i}{\partial r}\frac{\partial\psi_j}{\partial r}+k\frac{\partial\psi_i}{\partial z}\frac{\partial\psi_j}{\partial z}\right]d\Omega \qquad F_i=-\oint_{\Gamma_2}q\psi_i\,d\Gamma$$



Objective function:

$$S=\sum_{i=1}^{r}\left(Y_{m+i-1}-\hat{T}^{+}{}_{m+i-1}\right)^2$$

Flux computed from:

$$(\Delta q)_m=\frac{\sum_{i=1}^{r}\left[Y_{m+i-1}-\hat{T}_{m+i-1}\right]\phi_i}{\sum_{i=1}^{r}(\phi_i)^2}$$

Using Sensitivity Coefficient:

$$\phi_i=\frac{\left(\hat{T}^{+}{}_i-\hat{T}_i\right)}{\Delta q_i}$$

Modeling HTC during Quenching in Water*

*K Babu and T.S.Prasanna Kumar, Mathematical Modeling of Heat Flux during Quenching, Met Trans., Vol 41B, pp 214- 224, Feb 2010

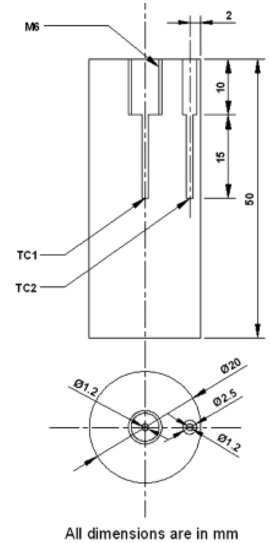


Fig. 1—Schematic of the quench probe.

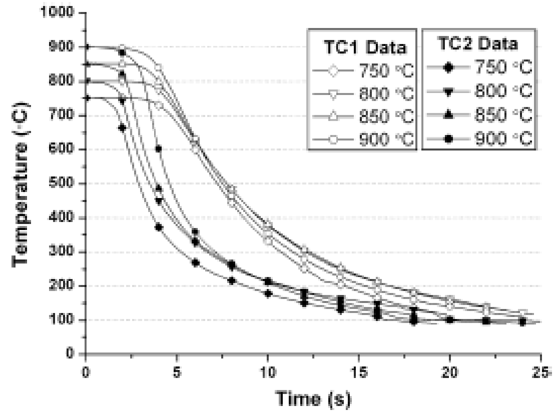


Fig. 3—Temperature data measured at TC1 and TC2 for the selected initial soaking temperatures.

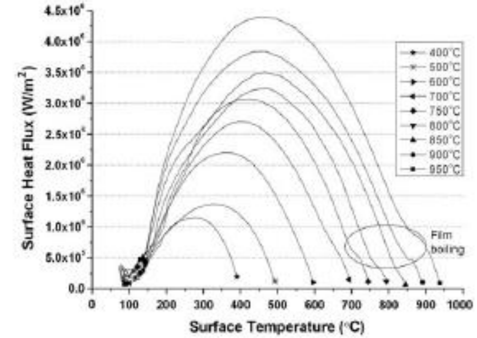


Fig. 11—Heat flux as a function of surface temperature for different initial soaking temperatures.

- Experiments showed that the heat flux rate is dependent on soaking temperature.
- From the model, the heat flux values at different surface temperature can be calculated.
- It is known that for large objects like gear wheels etc, the surface temperature varies depending on geometry (corners cool fastest)
- The heat flux model has two parts:
  - A model from the start of the quenching up to the peak and
  - A model from the peak to the end of quenching.

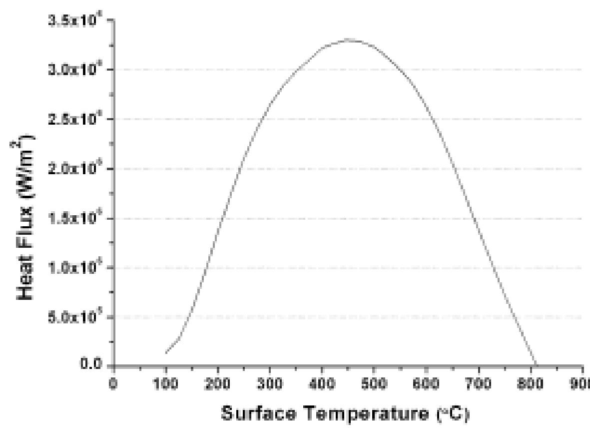
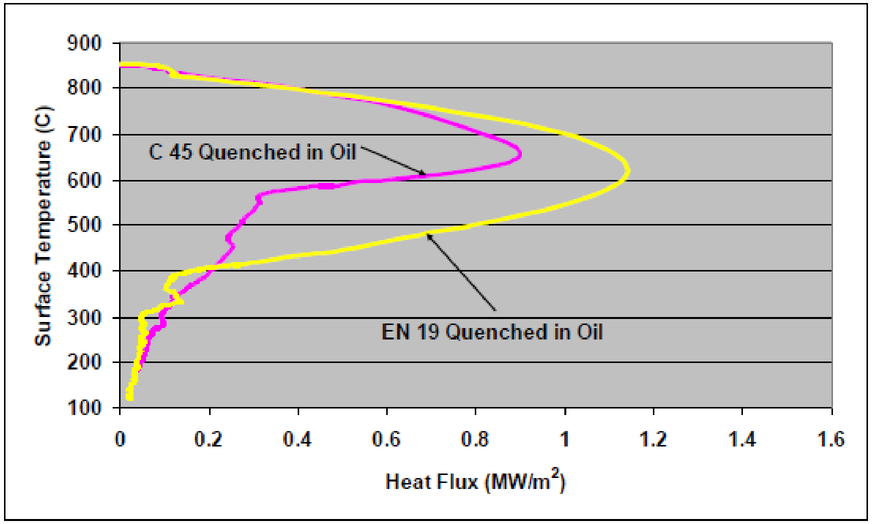
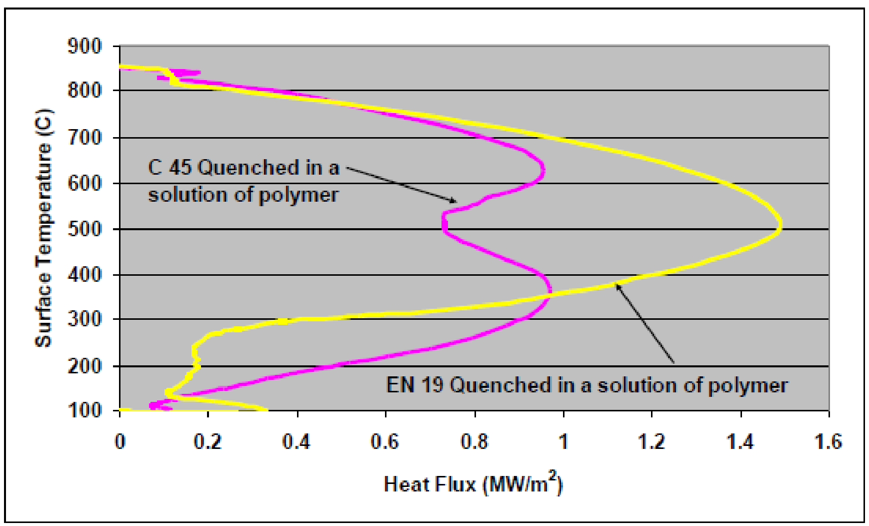


Fig. 16—Heat flux as a function surface temperature computed using the proposed model for 825 °C soaking temperature.

Need for Accurate Heat Transfer Modeling: Influence of Steel Grade on Heat Flux Rates*



Computed surface heat flux rates : **En19 and C45** quenched in **mineral oil**

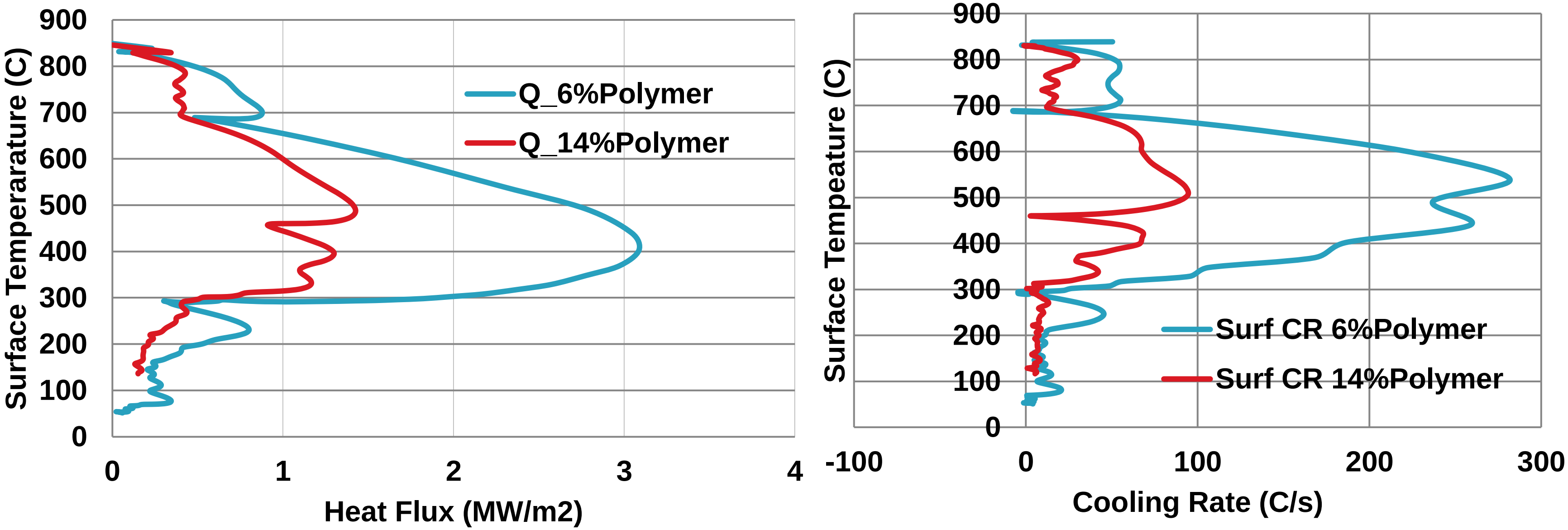


Computed heat flux rates : **EN19 and C45** quenched in an aqueous **polymer solution**

*T.S.Prasanna Kumar, 'Influence of Steel Grade on Surface Cooling Rates and Heat Flux during Quenching', JMEPEG _ASM International DOI: 10.1007/s11665-013-0552-9 1059-9495

Need for Accurate Heat Transfer Modeling: Influence of Polymer Concentration on Heat Flux and Cooling Rates

Results of quenching 41Cr4 in aqueous polymer solutions



Surface heat flux rate, cooling rate and austenite decomposition rates influence each other

Boiling Heat Transfer – A Summary

- Quenching is accompanied by boiling - complex heat transfer
- Heat transfer during quenching
  - affected by quench tank design (agitation levels and uniformity)
  - the type and state of quenchants(oxidation, contamination etc.)
- Necessary to measure HTC *in situ* for best results
- Reference Quench Probe is the tool
  - Based on Inverse Heat Transfer and metallurgical models
- Regression models for HTC are plant specific

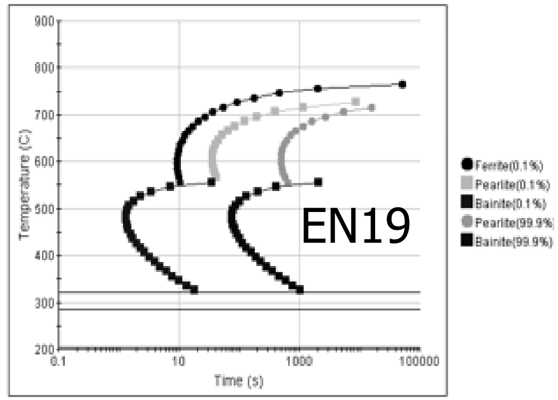
Estimation of As-Quenched Hardness

Abhaya Simha N. R, Sushanth M. P, Sachin V Bagali, Maruti, T. S. Prasanna Kumara, V. Krishna 'Estimation of hardness during heat treatment of steels' *Metal Science and Heat Treatment*, Vol. 61, Nos. 7 – 8, November, 2019 (Russian Original Nos. 7 – 8, July – August, 2019)
Translated from *Metallovedenie i Termicheskaya Obrabotka Metallov*, No. 7, pp. 51 – 58, July, 2019.A

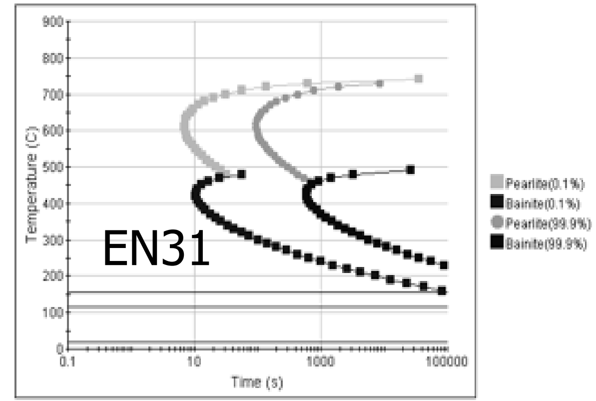
TABLE I. CHEMICAL COMPOSITION OF STEEL SPECIMENS

Steel	C	Si	Mn	Ni	Cr	Mo	V	CE*
C25	0.25	0.4	0.5	0	0	0	0	0.29
EN8	0.446	0.187	0.74	0	0	0	0	0.50
EN19	0.38	0.28	0.88	0.23	0.86	0.162	0	0.55
EN31	0.96	0.26	0.33	0.2	1.43	0.01	0	1.14
EN24	0.4	0.3	0.6	1.5	1.2	0.25	0	0.62

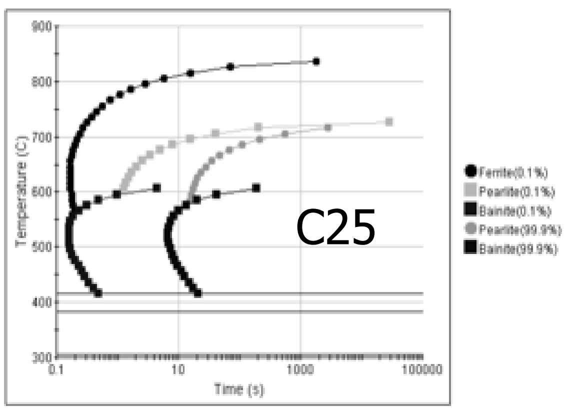
*CE = Carbon Equivalent calculated using
CE=C+Si/25+(Mn+Cu)/16+Ni/40+Cr/10+Mo/15+V/10



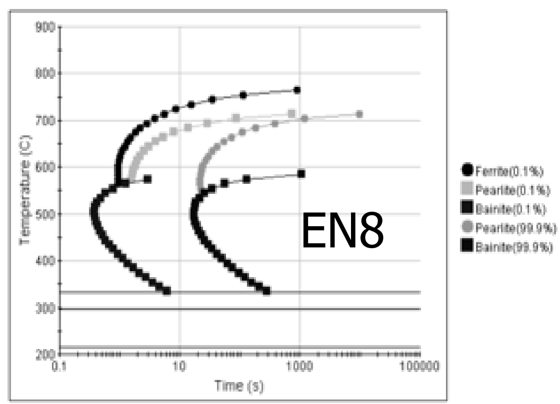
Grain size : 9 ASTM
Austenitisation : 821.72 C



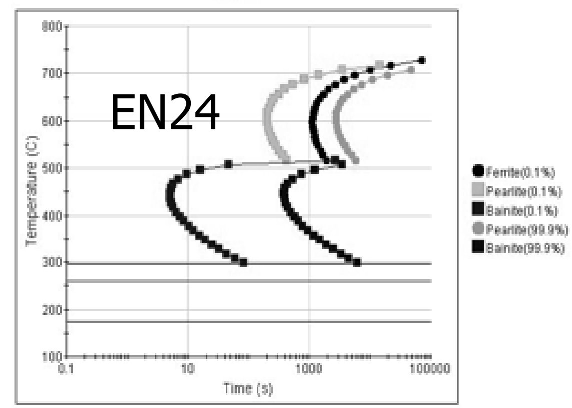
Grain size : 9 ASTM
Austenitisation : 860.0 C
Cementite 0.99 Austenite 99.01 Wt%



Grain size : 9 ASTM
Austenitisation : 891.85 C



Grain size : 9 ASTM
Austenitisation : 824.84 C



Grain size : 9 ASTM
Austenitisation : 797.81 C

Estimation of As-Quenched Hardness

Abhaya Simha N. R, Sushanth M. P, Sachin V Bagali, Maruti, T. S. Prasanna Kumara, V. Krishna 'Estimation of hardness during heat treatment of steels' *Metal Science and Heat Treatment*, Vol. 61, Nos. 7 – 8, November, 2019 (Russian Original Nos. 7 – 8, July – August, 2019) Translated from *Metallovedenie i Termicheskaya Obrabotka Metallov*, No. 7, pp. 51 – 58, July, 2019

Fig. 2. Image captured during end quenching

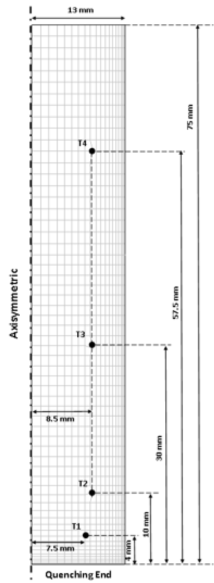
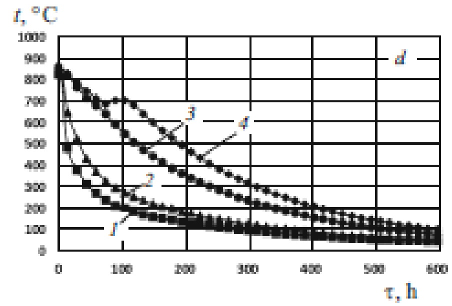
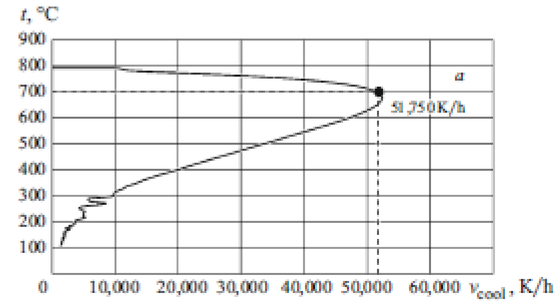


Fig. 4. Schematic representation of end quench specimen

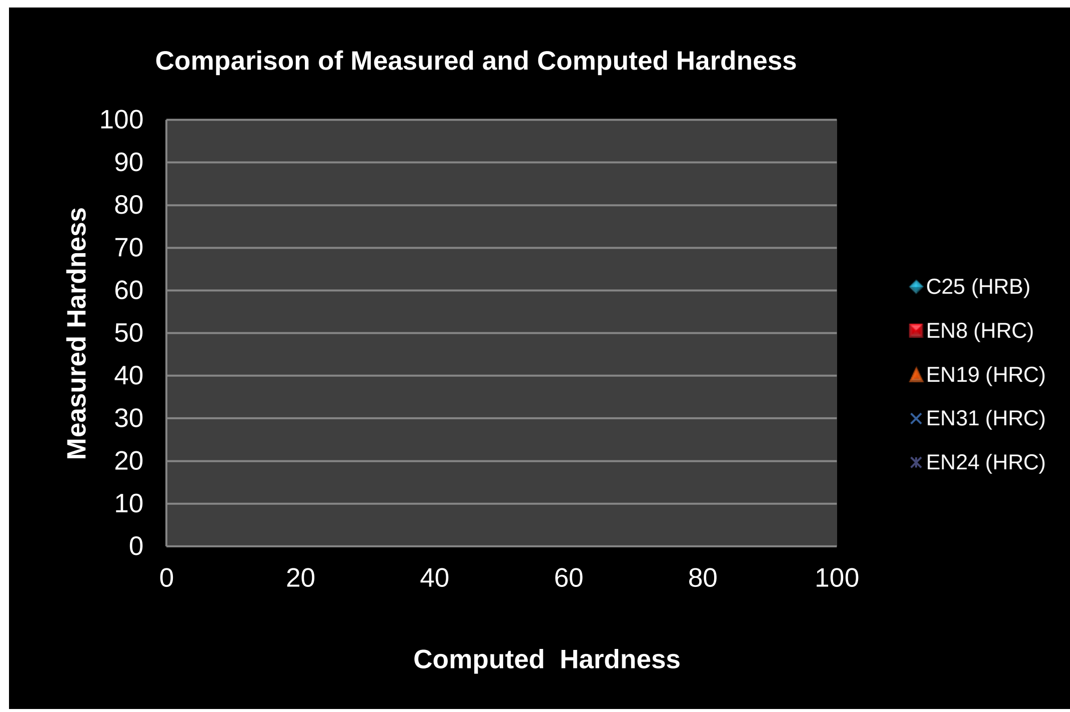




$$HV_M = 127 + 949C + 27Si + 11Mn + 8Ni + 16Cr + 21\log(V_r);$$

$$HV_B = -323 + 185C + 330Si + 153Mn + 65Ni + 144Cr + 191Mo + (89 + 53C - 55Si - 22Mn - 10Ni - 20Cr - 33Mo)\log(V_r);$$

$$HV_{FP} = 42 + 223C + 53Si + 30Mn + 12.6Ni + 7Cr + 19Mo + (10 - 19Si + 4Ni + 8Cr + 130V)\log(V_r).$$



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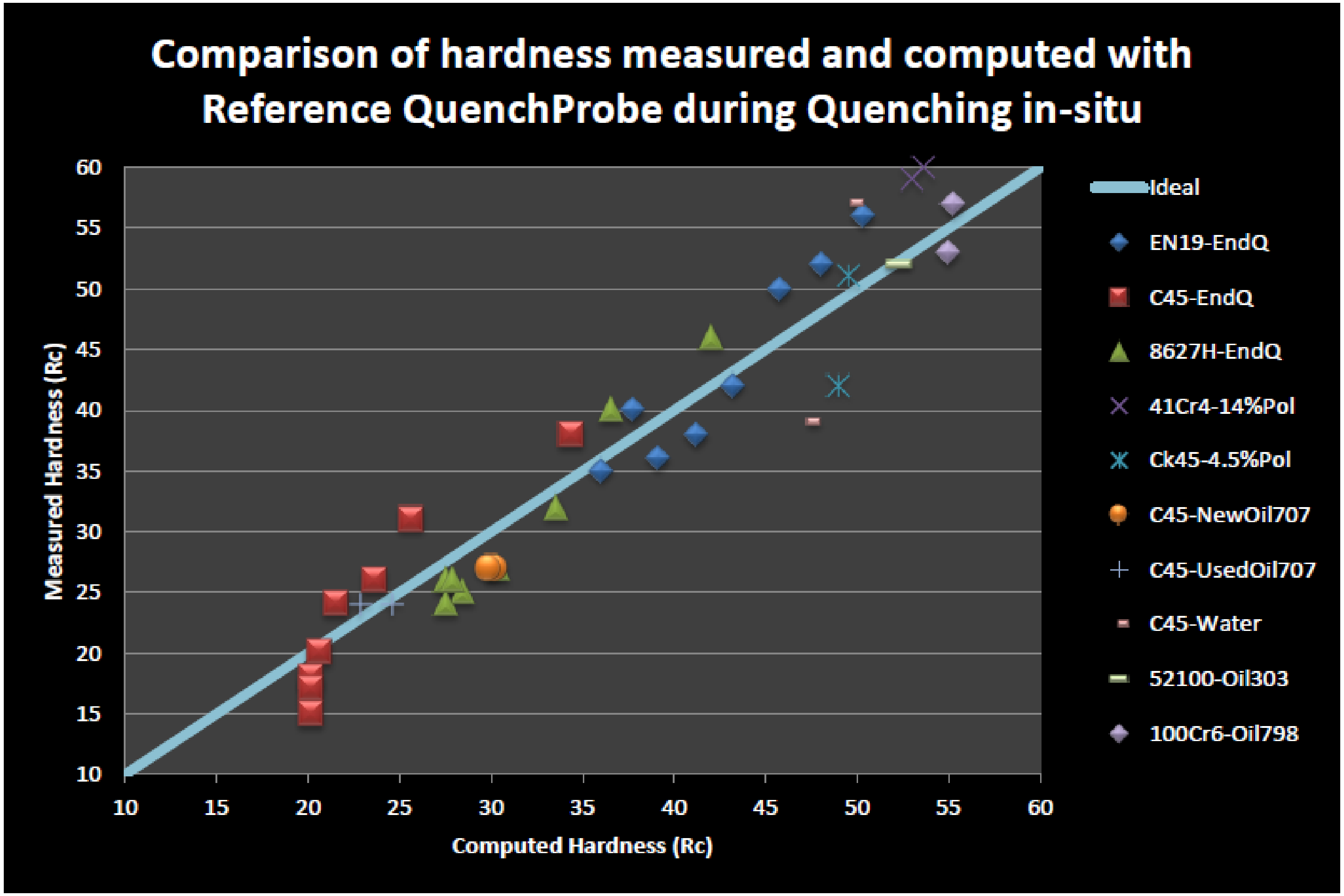
Estimation of As-Quenched Hardness – Industrial Trials with Different Quenchants



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Estimation of Tempered Hardness*

*R.A.Grange, C.R.Hribal and L.F.Porter, ‘Hardness of Tempered Martensite in Carbon and Low-alloy Steels’, Met. Trans A, Vol 8 A, Nov 1977, pp 1775-1785

Table I. Levels of Significant Elements in Iron-Carbon Alloys and High Cleanliness Steels Investigated

Alloy Series	Levels of Element Varied, Pct
Carbon*	0.12, 0.20, 0.42, 0.50, 0.72, 0.98
0.5Mn–Carbon*	0.08, 0.20, 0.42, 0.58, 0 78
0.2C–Manganese*	0.35, 0 64, 0.90, 1.22, 1 66, 1.95
0.2C–0.5Mn–Phosphorus*	0.002, 0.06, 0.28
0 19C–0.53Mn–Silicon*	0.09, 0.29, 0.56, 0.85
0.18C–0.30Mn–Nickel*	0.20, 0.27, 0.80, 1.55
0.19C–0.3Mn–Chromium*	0.1, 0.18, 0.40, 0.63
0.18C–0.3Mn–Molybdenum*	0.06, 0.12, 0.17, 0.41
0.19C–0.5Mn–Vanadium*	0.02, 0.052, 0.075, 0.18

*Element varied.

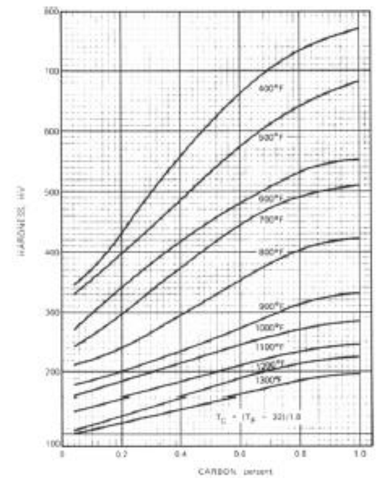
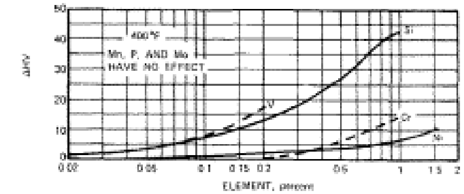
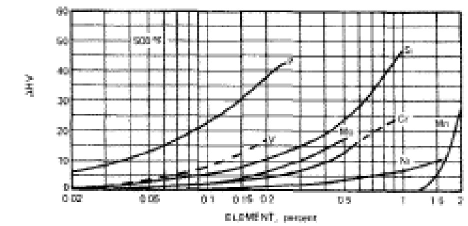


Fig. 7—Chart showing hardness of tempered martensite in Fe-C alloys.



8—Effect of elements on the hardness of martensite tem- ed at 400°F (204°C) for 1 h.



9—Effect of elements on the hardness of martensite tem- d at 500°F (260°C) for 1 h.

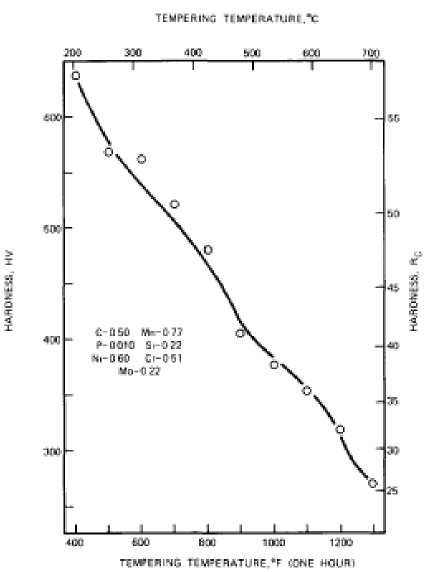


Fig. 19—Comparison of the measured (curve) and estimatec 8650

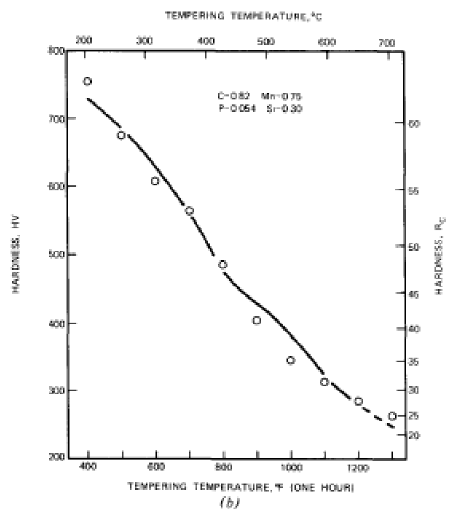


Fig. 18—(a) Comparison of measured and estimated hardness of tempered martensite in an AISI 1026 steel. (b) Comparison of measured and estimated hardness of tempered martensite in an AISI 1080 steel.

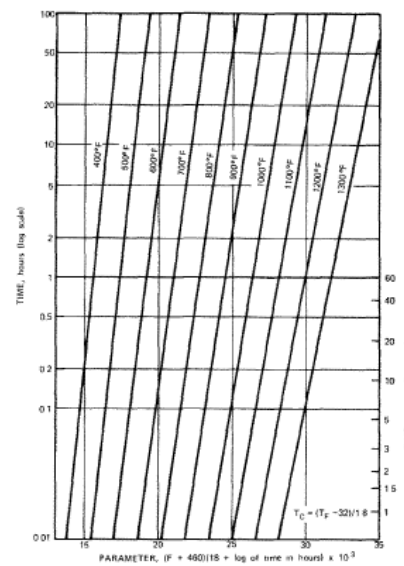
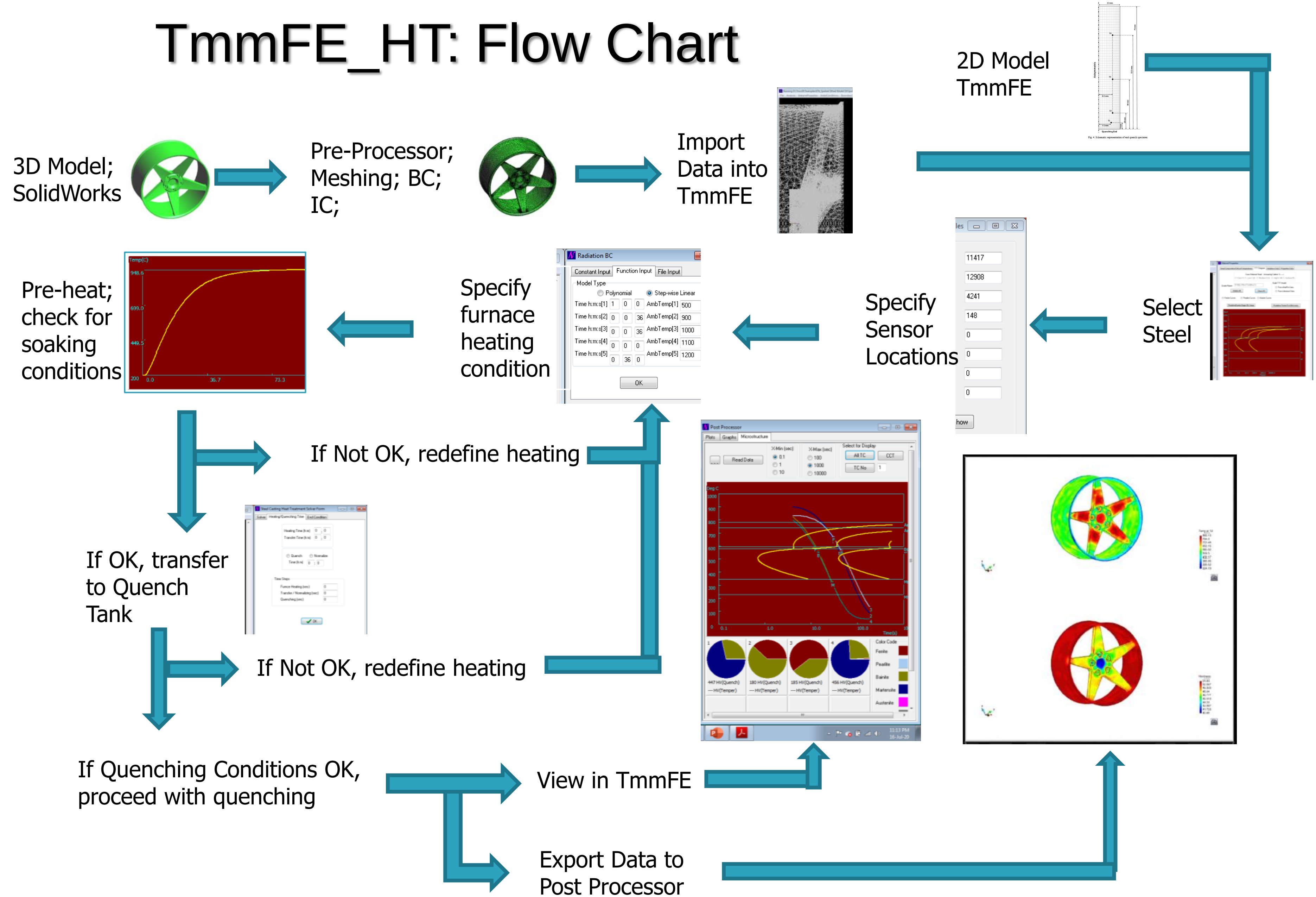


Fig. 21—Chart showing relationship of tempering parameter to temperature and time.

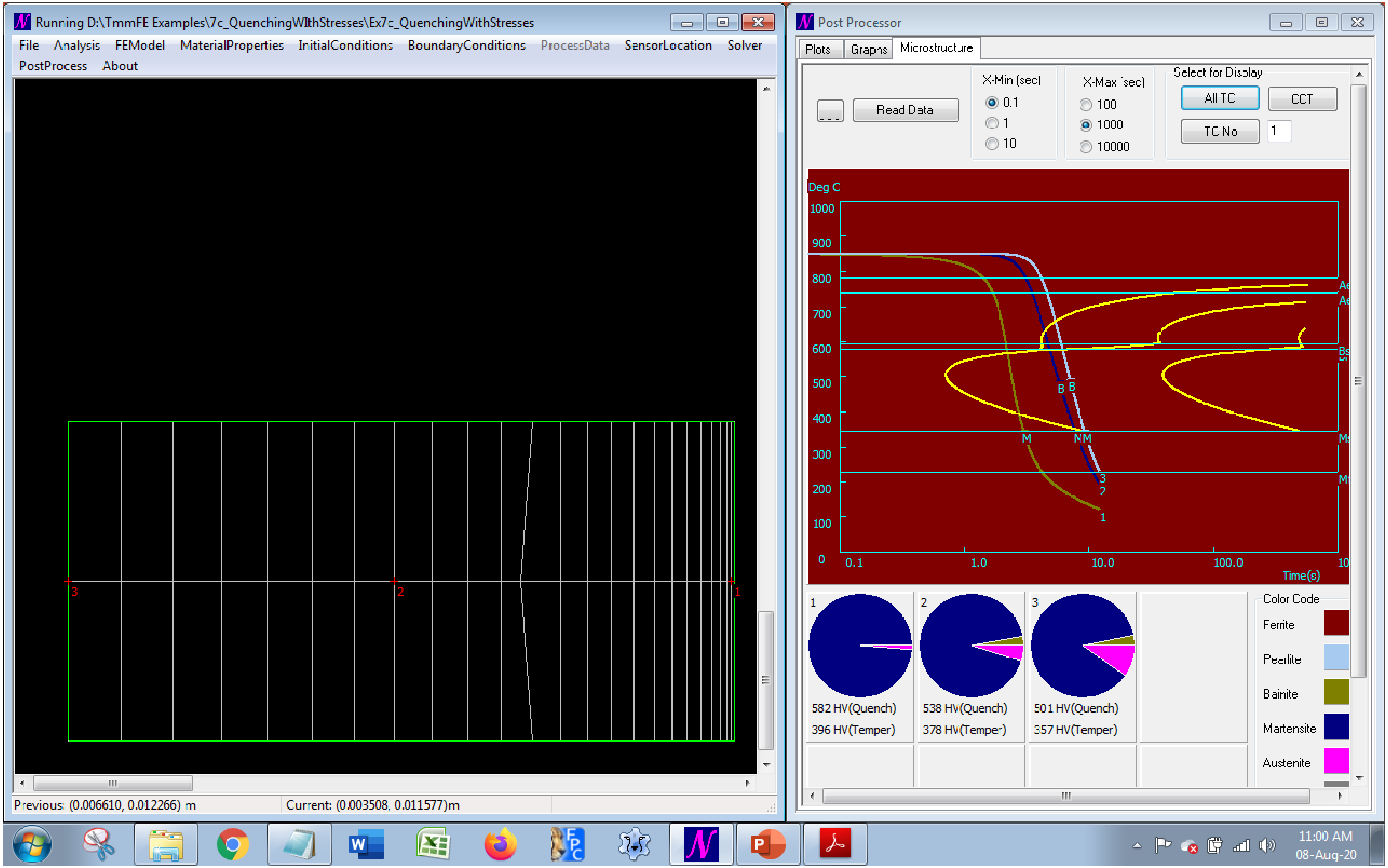
Tempered hardness is the sum of hardness of the base Fe-C alloy plus the contributions from all the alloying elements: Mn, Ni, Cr, Mo, V…..

Model Integration and Features of Simulation Software

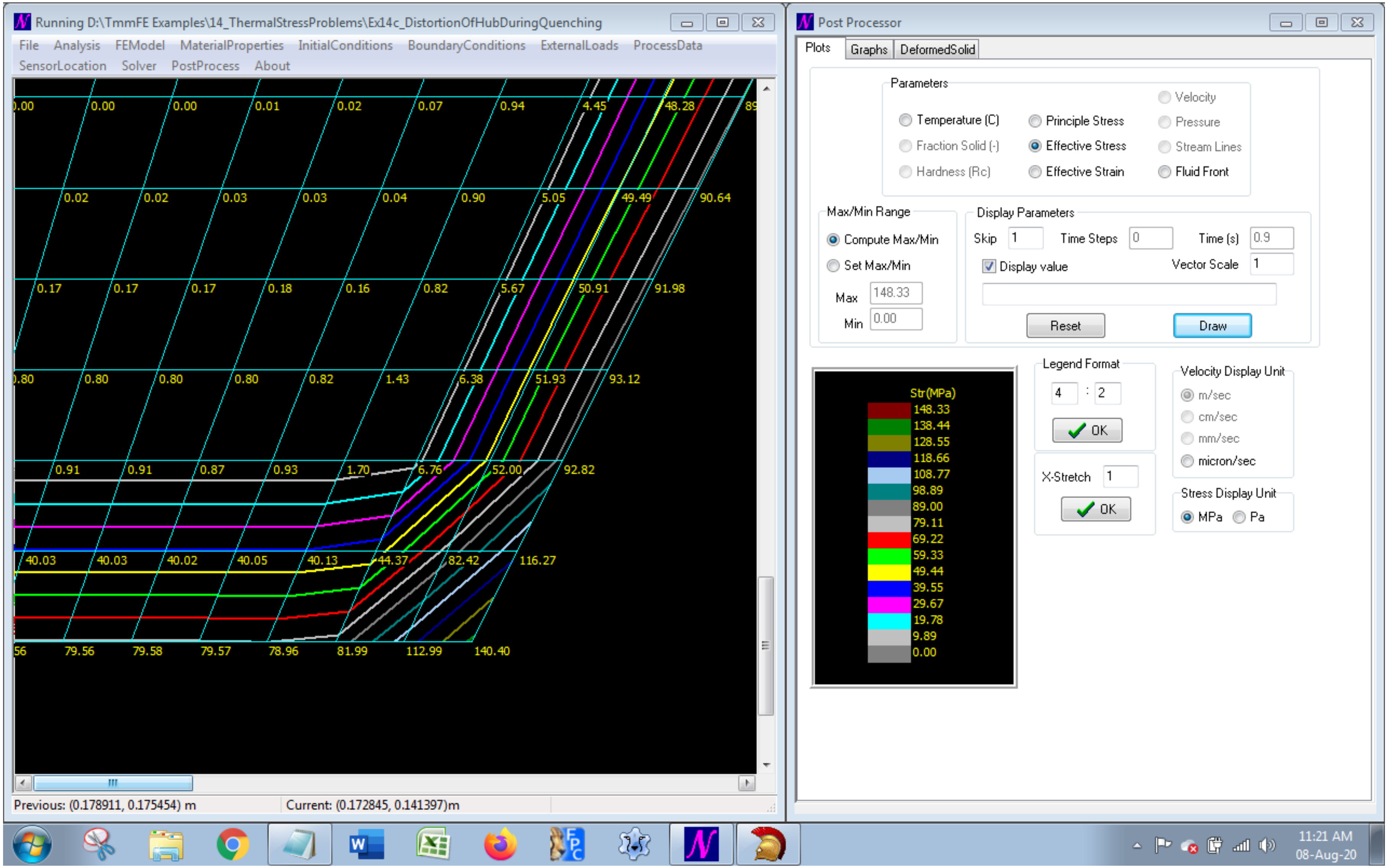
TmmFE_HT: Flow Chart



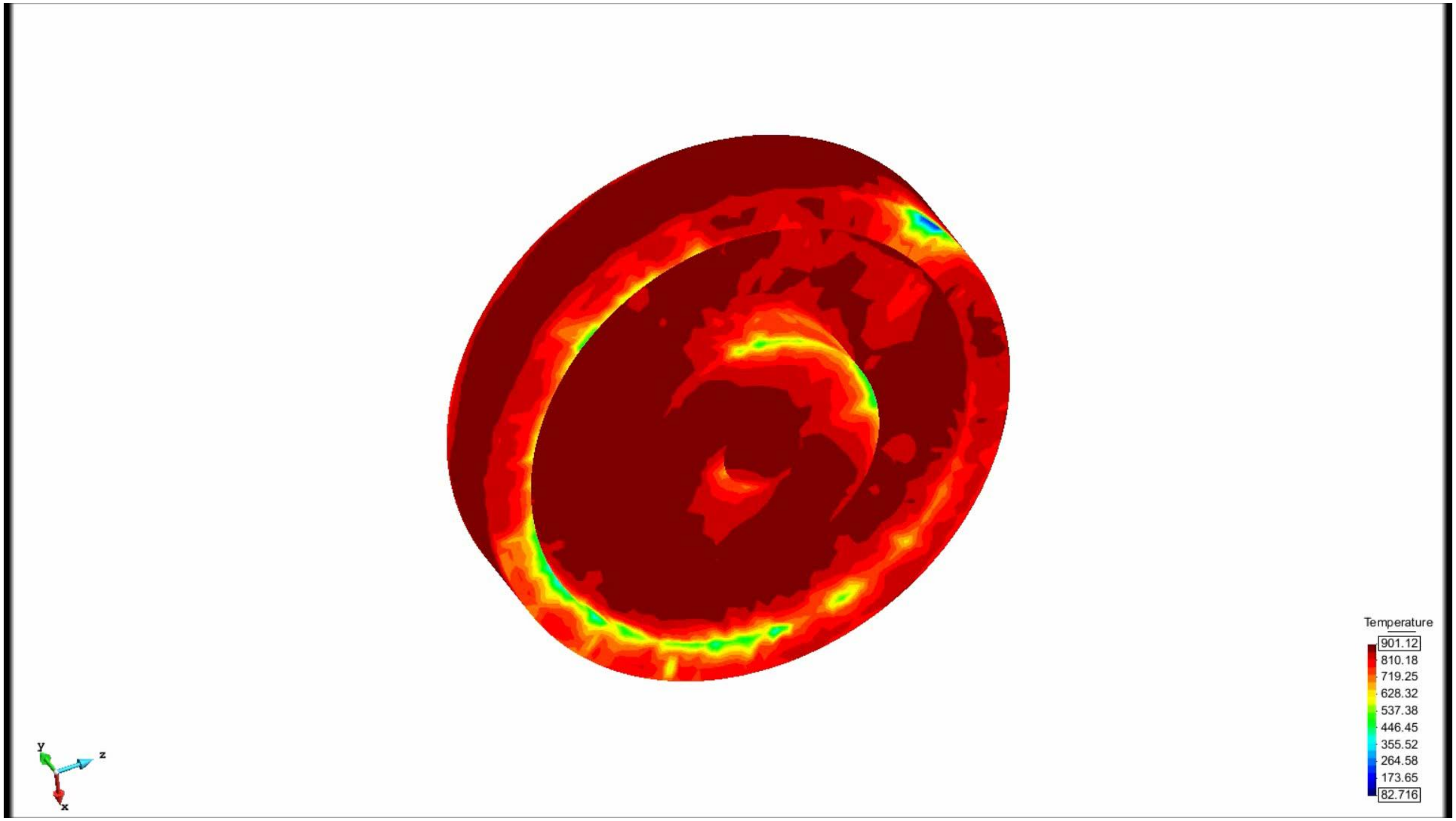
Post Processing -TmmHT



Stresses during Quenching



Post Processing - GiD



Industrial Case Studies

Industrial Consultancy / Case Studies

Sl No	Company
1	Ace Carbo Nitriders, Peenya
2	Automotive Axles Ltd, Mysore, India
3	Bharath Earth Movers Ltd., KGF, India
4	Bharath Forge Ltd., Pune, India
5	Caterpillar, Hosur
6	HAL, Bangalore, India
7	IndCarb, Attibele
8	L&T, Hazira, India
9	LVM, Bangalore, India
10	Mahindra Forge Ltd., Pune, India
11	NBC Bearings, Jaipur, India
12	SKF Bearings, Pune, India
13	SSS Springs, Siriperambudur, India
14	Tamilnadu Heat Treatment and Fettling Services, Hosur

Steels tested:

C45, 41Cr4, 100Cr6, 8822H, SA 542, 52100, 4140, SUP 9, ORVO, H13, DAC, MSSR 6503, AMS 6431, S99

Quenchants tested

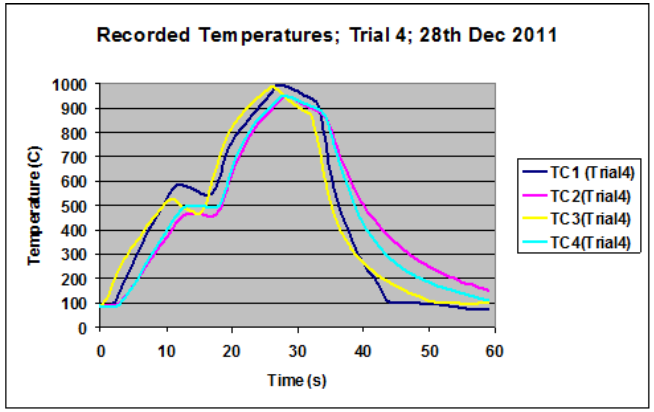
Servo 707, Castrol 798, Nippon 303, Hardcastle Polymer solutions (4.5%, 6.0%, 13.5%, 14.0%), Water
All in agitated tanks

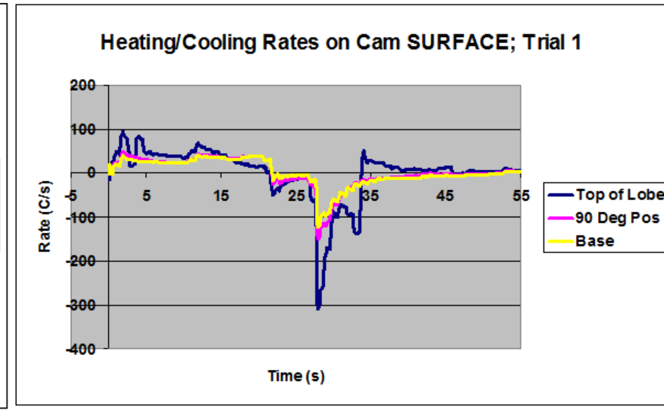
Gas Quenching

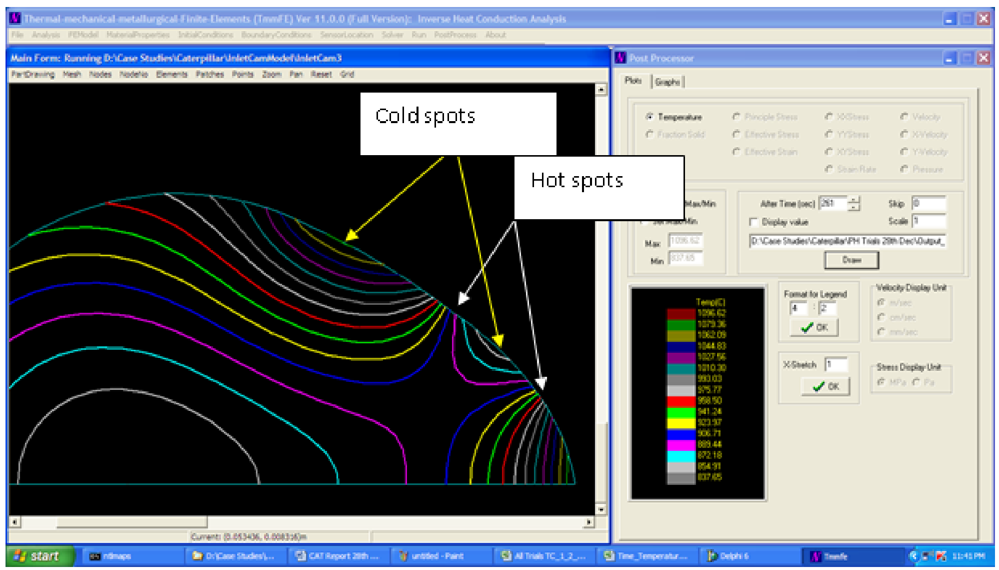
Lab trials in static quenchants

25 International Journal / Conference Publications / Presentations

Crack Elimination during IH of Cam Shafts



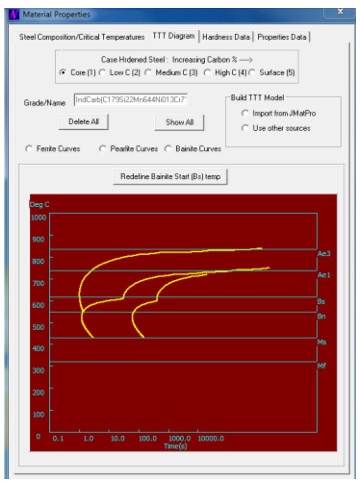


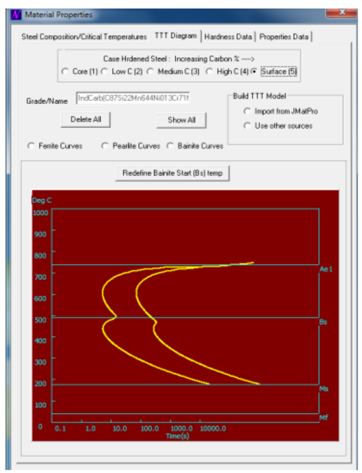


Lowering the concentration of PAG polymer was the solution

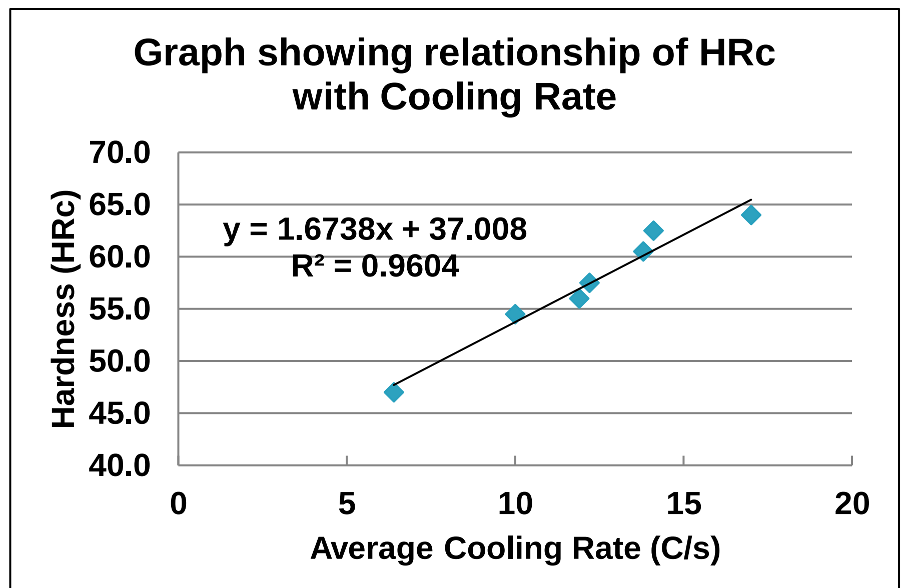
In-Situ testing of Case Hardened Steels

Zone	Th(mm)	%C
Core	6.50	0.179
Low carbon	1.50	0.215
Medium carbon	0.97	0.380
High carbon	0.76	0.650
Very high carbon	0.77	0.870

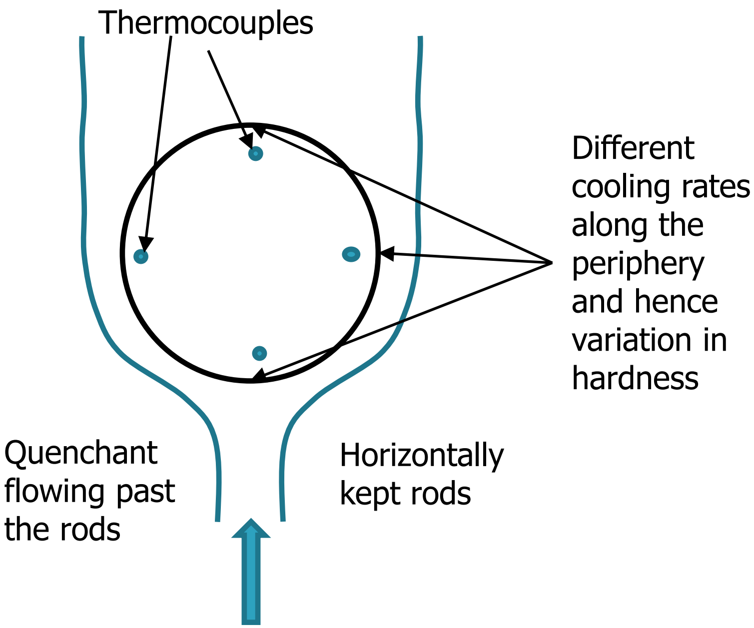




Test No		Furnace	Condition	Av CR (600-100)	Predicted HRc	Measured HRc	Error
Test 1		D	Agitated	10	53.7	54.5	0.8
Test 3		G	Agitated	12.2	57.4	57.5	0.1
Test 4		Bucket	New Oil	6.4	47.7	47.0	-0.7
Test 5		F	Agitated	11.9	56.9	56.0	-0.9
Test 6		F	Agitated	14.1	60.6	62.5	1.9
Test 7		F	Agitated	17	65.4	64.0	-1.4
Test 8		B	Agitated	13.8	60.1	60.5	0.4



Stacking Efficiency

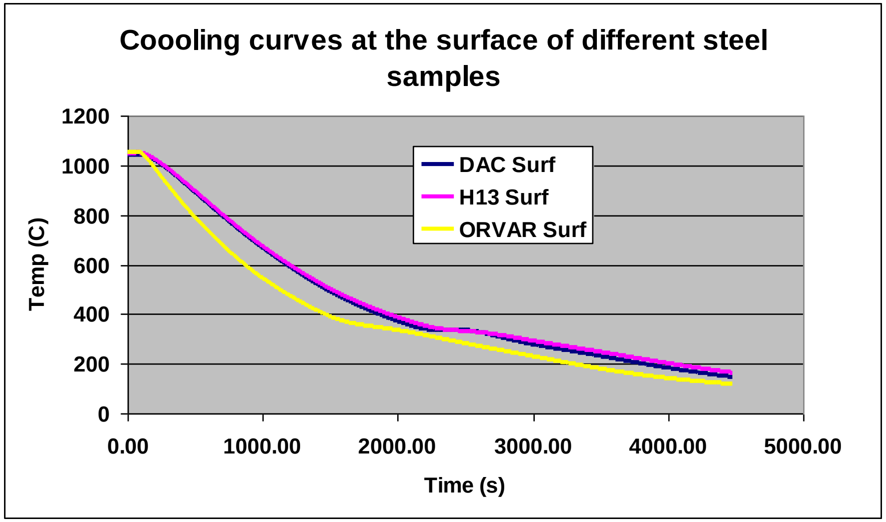


Schematic of the test rod (90 mm diameter) instrumented with four thermocouples

Sl No	Parameter	Top	Left	Bot'm	Right	Core
1	Maximum heat flux (MW/m^2)	1.50	3.40	2.97	1.84	-
2	Surface temperature at which Maximum heat flux occurs (C)	430.00	570.00	572.00	523.0	-
3	Maximum heat transfer coefficient (W/mK)	-	-	-	-	-
4	Surface temperature at which the maximum heat transfer coefficient occurs (C)	-	-	-	-	-
5	Maximum cooling rate (C/s)	73.00	320.00	269.00	119.00	13.6
6	Surface temperature at which the maximum cooling rate occurs (C)	673.00	569.00	572.00	523.00	680.00

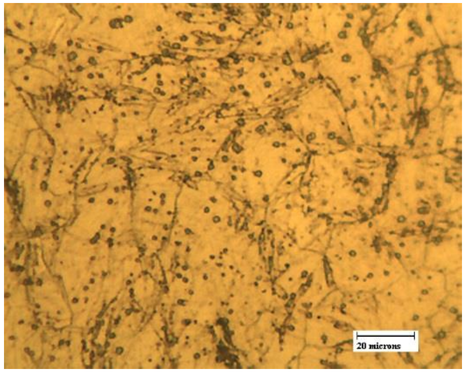
Location	Ferrite	Pearlite	Bainite	Martensite	Austenite	Hardness(Rc)
Top	0.02	0.00	0.37	0.58	0.03	44.89
Left	0.00	0.00	0.23	0.73	0.04	48.20
Bottom	0.00	0.00	0.42	0.55	0.03	45.14
Right	0.18	0.00	0.13	0.67	0.02	43.33
Core	0.26	0.15	0.59	0.00	0.00	25.21

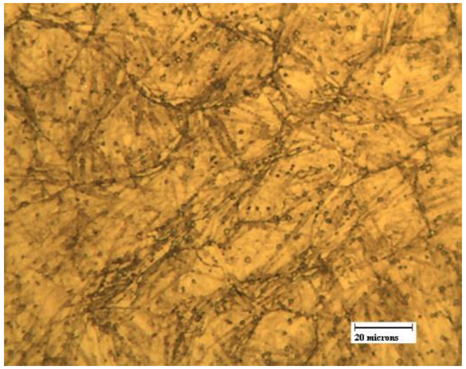
Vacuum Hardening of Tool Steels



Sl No	Sample ID	HRC	Microstructure (Volume %)			
			Carbide	Pearlite	Bainite	Martensite
1	DAC Surface	54.51	12.37	0.00	2.43	84.61
2	DAC Core	54.50	12.37	0.00	2.54	84.58
3	H13 Surface	54.49	12.47	0.00	2.57	83.65
4	H13 Core	54.50	12.22	0.00	2.42	84.22
5	ORVAR Surface	54.59	11.08	0.00	2.24	86.23
6	ORVAR Core	54.59	10.94	0.00	2.34	86.28

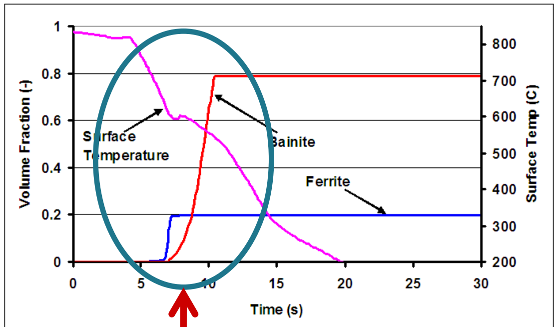
Sl No	Sample ID	HRC		Error %
		Measured	Computed	
1	DAC Surface	55.0	54.51	**-0.89**
2	DAC Core	54.7	54.50	**-0.37**
3	H13 Surface	55.0	54.49	**-0.93**
4	H13 Core	55.4	54.50	**-1.65**
5	ORVAR Surface	55.0	54.59	**-0.75**
6	ORVAR Core	55.7	54.59	**-2.03**

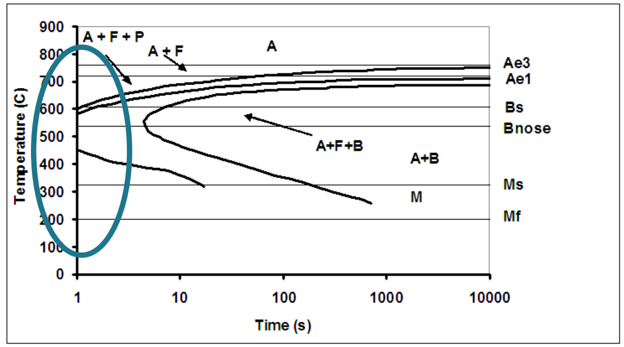


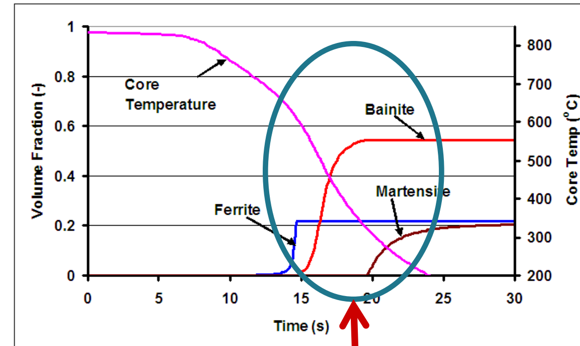


Uniformly distributed spheroidal carbide particles in a matrix of tempered martensite in ORVAR Supreme samples.
Left: Core; right: Surface

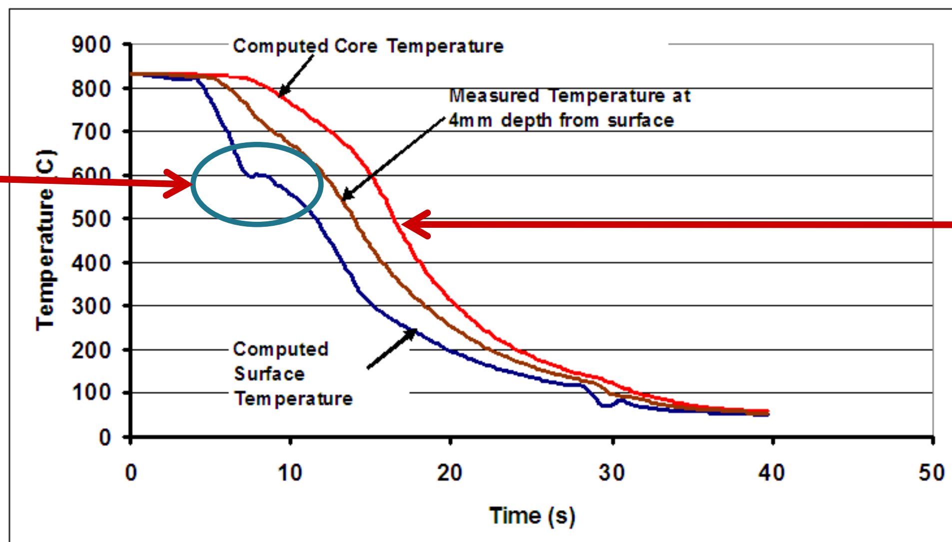
Anomalous Quenching of C45 in Oil (Harder core, Softer surface)







Surface re-heat resulting in early decomposition of austenite into 'softer' ferrite and bainite



Normal cooling at the core results in decomposition of austenite into martensite as well at lower temperatures

About TmmFE-HT

- Designed with the plant engineer in mind with the theory of heat transfer and metallurgical transformation working in the background.
- Integrates all processes during heat treatment from pre-heating to tempering
- Interface ensures smooth running of the software with inputs in practical terms.
- Robust algorithm combining features of both TTT diagram and the Equilibrium diagrams
- Reference Quench Probe – both in-situ and lab versions – indigenously designed, developed and tested in industries for measuring heat transfer coefficient / heat flux rate during quenching
- Heat transfer coefficient measured in-situ based on coupled inverse heat transfer and austenite transformation models - a unique feature.
- Model of HTC specific to steel and the plant conditions used for simulation for ensuring hardness estimation within 2-3 HRc.
- Surface cooling effects during transfer of large components from the furnace to the quench tanks are considered.
- Apart from end-to-end simulation TmmFE can be used for trouble shooting, selection of quenchants, defect elimination, improving stacking efficiency, monitoring of quenchnats etc.
- Saves energy during pre-heating by optimization of soaking time
- Two specialized modules tested extensively in laboratories and industries related to quench heat treatment.
- Helps to understand and optimize the Heat Treatment processes.
- For both (i) Metallurgical Engineers in industry and (ii) Researchers in Process Engineering and Mathematical Modeling

Acknowledgements

- It has been an unending journey for me into software development, equipment design and a never-lose-hope attitude in the past 37 years. I could not have reached this stage but for the support of:
- Prof O.Prabhakar, IIT Madras for initiating me into FEM software development way back in 1983 !
- My research students Mr Abhaya Simha, K.Babu, K. Arun Kumar, Prof K.V.Srinivasa Rao, Prof H.C.Kamath who validated my algorithms by experiments, to name a few
- Prof K.Narayan Prabhu for the challenges he has thrown me and with whom I have shared many Conference platforms
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- Prof H.Md.Roshan of Maynard Steels USA for the many discussions and his probing questions

Thanks for Your Attention