

Application Example:

Hardenability Design Using the Steel Model Library

Database(s):	FEDEMO, MFEDEMO	Module(s):	Steel Model Library
Version required:	Thermo-Calc 2021b or newer*	Calculator(s):	Martensite Temperatures Model, Martensite Fractions Model, Pearlite Model, Bainite Model, Ferrite Model*, TTT Diagram Model, CCT Diagram Model
Material/Application:	Steel / Materials Selection		
Calculation name:	PM_Fe_07_Hardenability_Design_of_Steel		

*The ferrite model was introduced in Thermo-Calc 2022b and terminal fractions were introduced in Thermo-Calc 2023a. The ferrite calculations are therefore not included prior to 2022b and the terminal fraction calculations are not included prior to 2023a.

INTRODUCTION

This example focuses on the hardenability design of steel using the <u>Steel Model Library</u> in Thermo-Calc. It shows how to find the optimal compositions for Fe–Mn–C steel to achieve high hardenability for the purpose of strength. Hardenability refers to the ability of steel to form martensite on quenching. It is a measure of the capacity of a steel to be hardened in depth when quenched from its austenitizing temperature. Among various factors, composition is one of the most important factors which has great influence on the hardenability of the steel. In this example, we use the Steel Model Library to investigate the possible composition ranges of Fe–Mn–C alloys to reach a fully martensitic microstructure.

To fulfil the requirement, room temperature martensite fraction should be large and the amount of retained austenite should be small. Meanwhile, other products of austenite decomposition should be avoided during continuous cooling. Such transformation products can be suppressed by fast quenching, yet the cooling rate is usually limited by the capacity of facilities or other problems such as cracking. Therefore, for hardenability purposes, it is desirable to achieve a fully martensitic structure with a relatively low cooling rate. This is done by promoting martensite formation while retarding other transformations through adjusting the steel composition.



How to Run the Calculation

If you have a license for Thermo-Calc 2021b or newer and a license for the Steel Model Library, you can follow along with this example in your software. Otherwise, you can read the PDF, which discusses the materials challenges and how Thermo-Calc can be used to solve them.

To run the calculation, open Thermo-Calc and navigate to the Help Menu \rightarrow Example Files... \rightarrow Property Models. This example includes one calculation file:

• **PM_Fe_07_Hardenability_Design_of_Steel:** uses the FEDEMO and MFEDEMO databases but requires a license for Thermo-Calc 2021b or newer and for the Steel Model Library.

Note: This calculation may take up to two days to run. We recommend using our recommended system requirements to run this calculation. See the <u>System Requirements page</u> on our website for more information.



See additional in-depth Application Examples available on our website.

Example File Results Differ from this Document

Beginning in Thermo-Calc 2024a, the calculation that is shipped with the software was simplified in order to speed up the simulation time. Therefore, if you run the calculation file included in the software, your plots will look slightly different from those shown in this Document. Even with the changes, the calculation may take over a day to complete.

The changes that were made are as follows:

- 1. Fe2Mn1C TTT calculator the Calculation setting was changed from Accurate to Quick
- 2. **Fe2Mn1C CCT calculator** the *Calculation setting* was changed from **Accurate** to **Quick**
- 3. **Fe3Mn0.7C CCT calculator** the *Calculation setting* was changed from **Accurate** to **Quick** and the number of steps was reduced from 20 to 10.

Calculation setting	Quick			
	Quick			
Calculation Type	Accurate			
	Custom			
Single One Axis Grid Min/Max Uncertainty Batch				
Grid Definitions				
Quantity Min	Max Number of steps			
Log10(cooling rate [K/s]) V -3.0	2.0 10 🗇			

Image 1. Shows the changes that were made to the **Fe3Mn0.7C CCT calculator** beginning in Thermo-Calc 2024a in order to speed up the simulation time. The Calculation setting was changed from **Accurate** to **Quick** and the number of steps was reduced from 20 to 10.



EXAMPLE CALCULATIONS AND EXPLANATIONS

Time-Temperature-Transformation (TTT) Diagram

High hardenability steel design means that the steel should have a high martensite finish temperature (Mf) or, in other words, a high martensite fraction at room temperature, and at the same time, a long starting time of formation of other austenite decomposition products such as ferrite, pearlite, and bainite. Figure 1 shows the calculated TTT diagram of a Fe–2Mn–1C (wt.%) steel using the Thermo-Calc Steel Model Library. Grain size is taken as 100 µm throughout this document. The arrows on the TTT diagram indicate the directions we should search towards for high hardenability, i.e., high temperatures for martensite to start (Ms) and form to a certain percentage (M50), as indicated by the yellow arrow, and long start times of pearlite, bainite, and ferrite, as indicated by the blue arrows. Using the TTT diagram is a simplified approach for hardenability analysis since the transformation kinetics is different under continuous cooling conditions.



Figure 1. Calculated TTT diagram of Fe–2Mn–1C (wt.%), which shows time-temperature curves for ferrite start (2%), pearlite start (2%), bainite start (2%), 50% and 98% austenite transformation, and the Ms and M50 temperatures for athermal martensite. Arrows in the diagram indicate directions towards high hardenability.



Martensite Fractions

In this section we investigate how Mn and C contents influence the amount of martensite at room temperature. Figure 2 shows the calculated Total Martensite Percentage as a function of Mn and C contents for an Fe–Mn–C system using the Martensite Fractions Property Model in the Thermo-Calc Steel Model Library. Three contour curves are shown, which correspond to 95%, 90%, and 80% of martensite respectively. According to the calculation results shown in Figure 2, increased concentration of either Mn or C leads to a decrease in martensite fraction. The region of interest for us, where the total martensite percentage is higher than 95%, has a Mn content lower than 4 wt.% and a C content lower than about 1.04 wt.%.



Figure 2. Total Martensite Percentage (80%, 90%, and 95%) as a function of Mn and C contents for Fe–Mn–C.



Pearlite Formation

From the TTT diagram in Figure 1 we can see that the nose of the start time of pearlite (corresponding to 2% of pearlite) of Fe–2Mn–1C (wt.%) is at a temperature around 800 K, which means that pearlite is most likely to begin forming within a short time at this temperature. We then calculated the pearlite start time when varying both Mn and C contents at a temperature of 800 K. We use the Pearlite Property Model for this calculation because it runs faster than the TTT Diagram Model. The result is presented in Figure 3 as contour curves of pearlite start times equal to 5 s, 10 s, 20 s, and 100 s respectively, as a function of Mn and C concentrations. As can be seen, increasing Mn content retards the formation of pearlite. On the other hand, the effect of C on the pearlite start time is not monotonic.



Figure 3. Start time of pearlite formation (2% pearlite, unit: second) as a function of Mn and C contents for Fe–Mn–C at 800 K.



Bainite Formation

From the TTT diagram in Figure 1 we can also see that the shortest start time of bainite (corresponding to 2% of bainite) of Fe–2Mn–1C (wt.%) is at a temperature around 700 K. For this composition, bainite is predicted to start shortly after pearlite, so it is not the product that controls hardenability. But in order to keep track of the bainite formation kinetics, we also calculated the bainite start time when varying both Mn and C contents at a temperature of 700 K. We use the Bainite Property Model for this calculation because it runs faster than the TTT Diagram Model. Figure 4 shows the result as contour curves of bainite start times equal to 5 s, 10 s, 20 s, and 100 s respectively, as a function of Mn and C concentrations. As can be seen, increasing Mn and C contents retards the formation of bainite.



Figure 4. Start time of bainite formation (2% bainite, unit: second) as a function of Mn and C contents for Fe–Mn–C at 700 K.

Ferrite Formation

Usually, proeutectoid ferrite should be considered for hypoeutectoid compositions (i.e. carbon content lower than the eutectoid composition, about 0.8 wt.%). From Figure 1 we can see ferrite barely appears, which is expected because the carbon content (1 wt.%) is quite high for ferrite to form. But we can choose to monitor ferrite start time at 900K in the composition space as a precaution. Figure 5 shows the contour curves of ferrite start times. For simplicity, we choose



paraequilibrium (PE) mode for ferrite. As can be seen, increasing Mn and C contents also retards the formation of ferrite.



Figure 5. Start time of ferrite (2%, unit: second) as a function of Mn and C contents for Fe–Mn–C at 900 K.

Note: The ferrite model was introduced in Thermo-Calc 2022b. The ferrite calculations are therefore not included prior to 2022b.



Composition Selection

As we need to consider both martensite fraction and the formation kinetics of pearlite, bainite, and ferrite, we merge Figures 2–5 into one plot, which is presented as Figure 6. The allowable region of compositions to achieve high hardenability is indicated by the yellow area in Figure 6. Within this composition range, we have more than 95% of martensite at room temperature, the start time of pearlite formation at 800 K is longer than 100 s, and the start time of bainite formation at 700 K is also longer than 100 s, which supposedly implies that the pearlite and bainite transformations are sufficiently slow under practical cooling conditions. Ferrite is apparently not controlling hardenability in this case. We can empirically choose Mn content lower than 4% to avoid processing issues.

We can then draw our conclusion that based on the above calculations, the composition that we should consider for achieving high hardenability in Fe–Mn–C steel has been narrowed down to the allowable region indicated in Figure 5, having 2.2–4 wt% Mn and 0.4–0.8 wt% C. The allowable composition that has the lowest Mn content is about Fe–3Mn–0.7C.



Figure 6. Total martensite percentage, start time of pearlite formation (2% pearlite, unit: second), and start time of bainite formation (2% bainite, unit: second), and start time of ferrite formation (2% ferrite, paraequilibrium mode, unit: second) as a function of Mn and C contents for Fe–Mn–C (merge of Figures 2–5).



Finally, we calculate the CCT diagrams and terminal fractions of transformation products for the two compositions before and after optimization, using the CCT Diagram Property Model. We set cooling profiles to start from 1000K and end at 298K. The CCT diagrams are shown in Figure 7 and terminal fractions in Figures 8 and 9. CCT diagrams provide transformation temperatures at different cooling rates, while terminal fraction plots provide details about the ending microstructure when transformations are complete or the ending temperature (298K) is reached. As is expected, Fe– 3Mn–0.7C has a higher martensite fraction at room temperature than Fe–2Mn–1C. Fe–3Mn–0.7C also requires a lower cooling rate (by a factor of 4 or above, as Figure 9 suggests) to reach an equal amount of martensite than Fe–2Mn–1C. Therefore, our calculations support that Fe–3Mn–0.7C has a higher hardenability than Fe–2Mn–1C.



Figure 7. Calculated CCT diagrams for Fe–2Mn–1C in the left plot and Fe–3Mn–0.7C in the right plot.



Figure 8. Calculated terminal fractions of transformation products for Fe–2Mn–1C in the left plot and Fe–3Mn–0.7C in the right plot.





Figure 9. Comparing terminal fractions of martensite of Fe–2Mn–1C and Fe–3Mn–0.7C. The latter exhibits a higher hardenability in that (1) the maximum martensite fraction is higher and (2) the cooling rate required to obtain an equal amount of martensite is lower.

Notes about the Example

A Continuous Cooling Transformation (CCT) diagram, which records the progress of the transformation of a material as it is cooled over a range of cooling rates, is more practical for hardenability design but slower to run. TTT diagrams can be used as a rough guide and provide a good starting point for the examination of hardenability. One problem with using a crossplot like Figure 6 is the possibility of changing nose temperature. One solution is to consider start times at several temperatures for each transformation product.