Pure Heat Conduction, Multizone and Isothermal Case

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The improvement of the solidification processes is very interesting for the Metallurgical Industry due to its high cost and difficulty. Each year they invert huge amounts of money to investigate in this field. That's the reason why in the last years the use of computers to simulate the processes have become very important, letting the companies reduce the number of the expensive experiments to test new methods or materials. Thanks to the high accuracy of the power simulation computer tools is possible to investigate in laboratories without wasting energy (i.e., energy needed to melt metals), leading to a reduction of the costs for the company and saving energy for the environment.

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1 Introduction

Several decades ago it was quite difficult to predict what was going on when a metal solidifies. Nowadays and thanks to the high calculation capacity of computers we can simulate with a high accuracy the solidification process of metals.

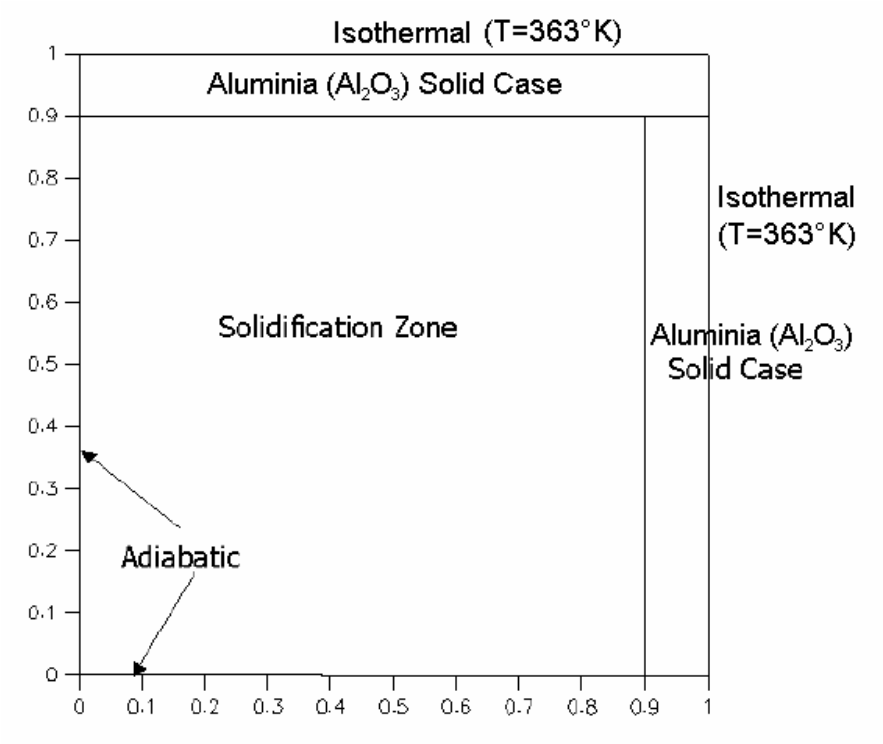
In particular this simulation has been done by using CFD-ACE+, a computational fluid dynamics program which has very powerful simulation tools.

2 Program description

CFD-ACE+ is a set of computer programs for multi-physics computational analysis. The programs provide an integrated geometry and grid generation module (CFD-GEOM), a graphical user interface for preparation of the model (CFD-GUI), a computational solver for performing the simulation (CFD-ACE(U)), and an interactive visualization program for examination and analysis of the simulation results (CFD-VIEW).

The program has many different modules for each type of calculation (flow, heat, turbulence, radiation…), being possible to use different modules at the same time. The ability to perform heat transfer analysis is an integral part of the CFD-ACE(U) solver. The program can be used to simulate many types of heat transfer problems. The simplest are pure heat conduction problems (this case). More advanced applications will add the simulation of flow. Ultimately the Heat Transfer Module solves for the energy in the system and can therefore be used to produce the temperature field energy transfer characteristics of the model.

3 Problem description



We have simulated the solidification process of a 2D box with two different metals, Aluminium and Iron in order to compare the differences between these two materials. The box has the following properties:

- Square 10x10 cm.
- Top and right walls are Isothermal (T=363°K). Wall width = 1 cm.
- Crucible material: Aluminia (Al_2O_3). Physical properties of the material needed for the simulation (Data given by Morgan Advanced Ceramics):

	Value	***Units***
Density	3850	*kg/m3*
Specific Heat	900	*J/(kg*K)*
Heat Conductivity	25	*W/(m*K)*

- Bottom and left walls are Adiabatic (heat transfer = 0).

As we will see below, Iron and Aluminium have very different physical properties values so it's quite difficult to compare them when, for example, Aluminium has a melting temperature of 933,25°K and for Iron is 1808°K. What I had done is equalize the heat quantity the metals have to remove during the solidification. So we have the following:

$$Q_{T_0 \to T_S}\Big|_{Fe} = Q_{T_0 \to T_S}\Big|_{Al}$$

$$m_{Fe} \cdot Cp_{Fe} \cdot \Delta T = m_{Al} \cdot Cp_{Al} \cdot \Delta T$$

$$V \cdot \delta_{Fe} \cdot Cp_{Fe} \cdot \left(T_0 - T_{S(Fe)}\right) = V \cdot \delta_{Al} \cdot Cp_{Al} \cdot \left(T_0 - T_{S(Al)}\right)$$

where,
- m: mass [kg]
- Cp: specific heat at 293°K
- V: volume
- δ: density
- T_0: initial temperature
- T_S: solidification temperature

Now we can simplify the equation setting ΔT for Iron in 100° (so T_0 for Fe will be 1908°K) and we also know that the volume is always the same. We substitute the variables for the values:

$$7874\left[kg/m^3\right] \cdot 490\left[J/(kg \cdot K)\right] \cdot 100 = 2702\left[kg\right] \cdot 900\left[J/(kg \cdot K)\right] \cdot \left(T_0 - 933.25\left[K\right]\right)$$

$$T_0 = 1091.91°K \approx 1092°K$$

$$\Delta T = 158.66°$$

So the simulation for the solidification process will start at 1908°K and 1092°K for Fe and Al, respectively. The two metals will transfer the same heat quantity and we will be able to compare them and see how much influence the other physical parameters such as the specific heat or the thermal conductivity in the solidification.

4 Calculations

4.1 Equations solved

Here I describe the mathematical equations used by CFD-ACE(U) and its Heat Transfer Module. Heat transfer processes are computed by solving the equation for the conservation of energy. This equation can take several forms and CFD-ACE(U) numerically solves the energy equation in the form known as the total enthalpy equation. This form is fully conservative and is given in the next equation.

$$\frac{\partial(\rho h_o)}{\partial t} + \nabla\bullet(\rho\vec{\nabla} h_o) = \nabla\bullet(k\nabla T) + \frac{\partial p}{\partial t} + \left[\frac{\partial(u\tau_{xx})}{\partial x} + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z}\right] + \left[\frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{yy})}{\partial y} + \frac{\partial(v\tau_{zy})}{\partial z}\right] + \left[\frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(w\tau_{zz})}{\partial z}\right] + S_h$$

where,

h_o = the total enthalpy and is defined as

$$h_o = i + \frac{p}{\rho} + \frac{1}{2}(u^2 + v^2 + w^2)$$

i = the internal energy and is a function of the state variables ρ and T

k = the thermal conductivity of the material

p = the static pressure

τ_{ij} = the viscous stress tensor which is

4.2 Calculations for Aluminium

First of all we describe the physical properties of Al needed for the simulation. In order to get a more realistic solution, CFD-ACE(U) lets the user to introduce the required inputs in different ways. We had used the next evaluation methods: *Constant*, for constant values, and *Piecewise Linear in T*, linear interpolation of specified variable versus T data.
(for more details, look at Q:\agspitz\cfdrc\Mia\Aluminium data)

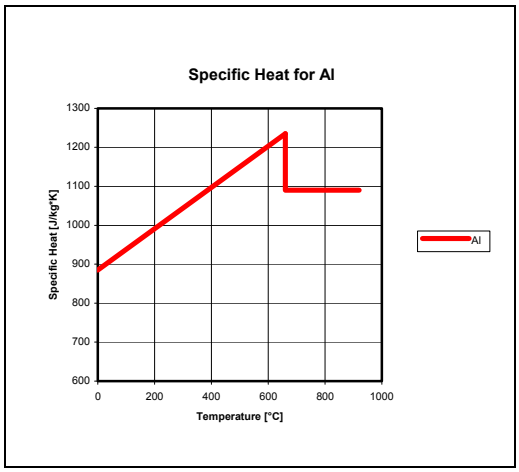
Required input values:

- *Density:* 2702 kg/m3
- *Latent heat:* 399903 J/kg
- *Solidification temperature:* 933,25 °K (660,25 °C)
- *Initial temperature of the solidification zone:* 1092°K
- *Temperature of isothermal Aluminia walls:* 363°K

- *Specific Heat:*

Temp [°K]	*Cp [J/(kg*K)]*
273	885
933,25	1235
933,35	1090
1193	1090

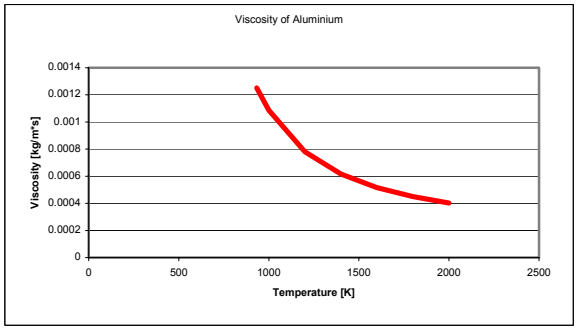
Specific heat vs. temperature diagram→



- *Viscosity (dynamic):*

Temp [°K]	*v [kg/(m*s)]*
933.25	1.25103633
1000	1.08549099
1200	0.77980016
1400	0.61571715
1600	0.51573867
1800	0.44934353
2000	0.40243665

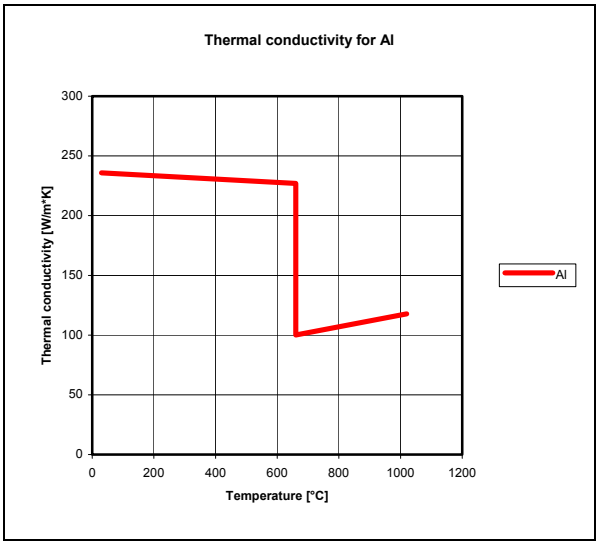
Viscosity vs. temperature diagram→



- *Thermal conductivity:*

Temp [°K]	*Tc[W/(m*K)]*
303	235.8846
933,25	226.91396
933,35	100.13612
1293	117.8072

Thermal conductivity vs. temperature diagram→



Another very important thing are the numerical parameters used to solve the simulation. The table below shows which ones I had used:

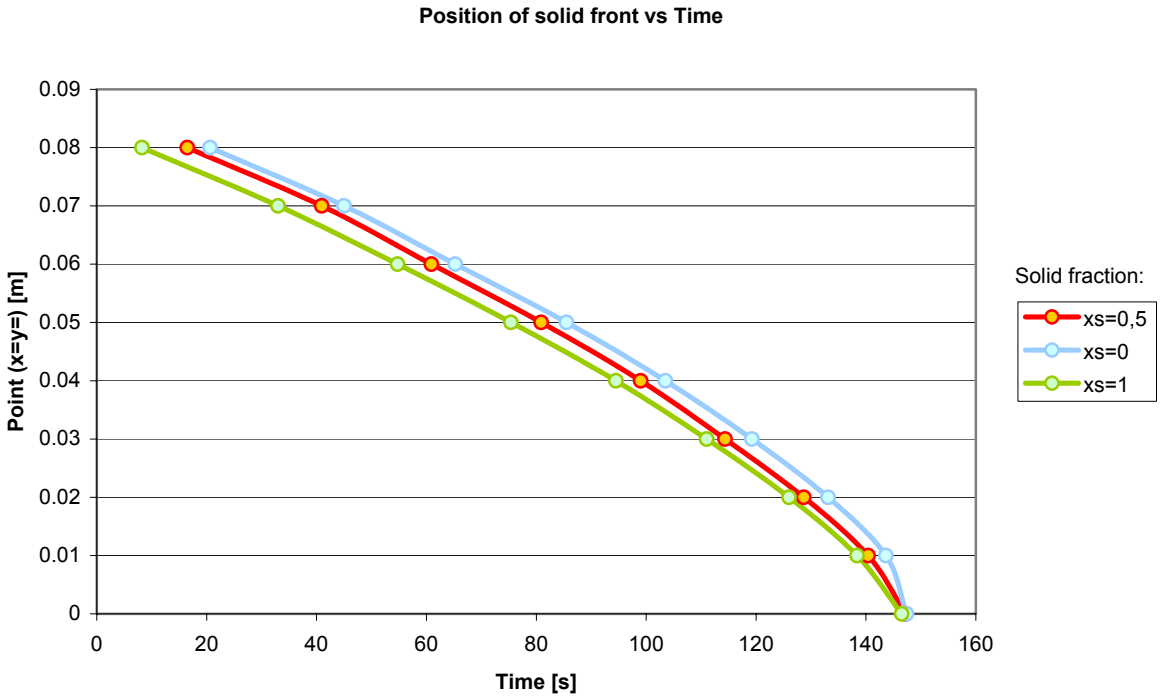
SOLVER CONTROLS

Iter	Shared	Max. Iterations	*1000*
		Convergence Crit.	*0.00001*
		Min. Residual	*1E-18*
Spatial	Spatial Differencing	Enthalpy	*Upwind*

Solvers	Solvers	Enthalpy	*CGS+Pre*	*2500*	*0.00001*
Relax	Inertial Relaxation	Enthalpy	*0.5*		
	Linear Relaxation	Temperature	*0.2*		
Limits		Enthalpy	*-1E+20*	*1E+20*	
		Temperature	*1E-10*	*5000*	
Adv	Heat transfer	CFL Relaxation	*Disabled*		

For more information about the input numerical parameters, please look at *CFD-ACE(U) User Manual – Chapter 12: Numerical Parameters*.

After the simulation, I obtained the following results:



The way I had obtained this diagram and the conclusions of the simulation are explained below. (for more details and information about the diagram and the data, look at Q:\agspitz\cfdrc\Mia\Case\Al+Aluminia crucible)

4.3 Calculations for Iron

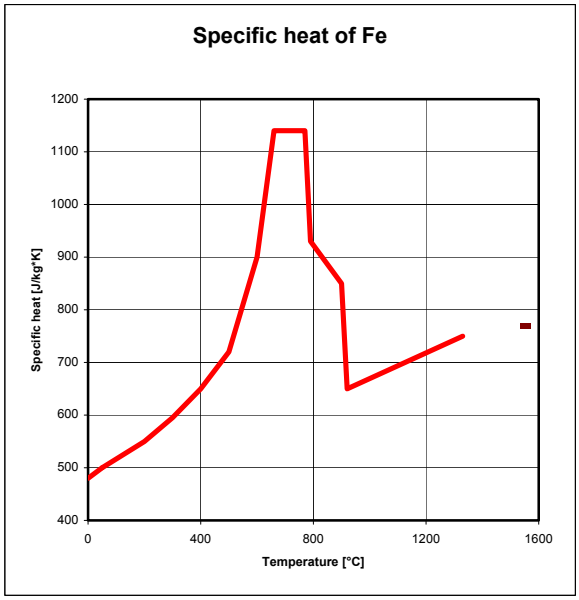
Here I'm doing the same as I had done with the Aluminium calculations. I entered all these physical properties of the material:
(for more information, look at Q:\agspitz\cfdrc\Mia\Steel and Iron data)

Required input values:

- *Density:* 7874 kg/m3
- *Latent heat:* 530769.23 J/kg
- *Solidification temperature:* 1808 °K (1535 °C)
- *Initial temperature of solidification zone:* 2000 °K (1827 °C)
- *Temperature of isothermal Aluminia walls:* 363°K

- *Specific heat:*

Temp [°K]	*Cp [J/(kg*K)]*
273	480
323	500
473	550
573	595
673	650
773	720
873	900
933	1140
1043	1140
1063	930
1173	850
1193	650
1603	750
1808	770
2273	770

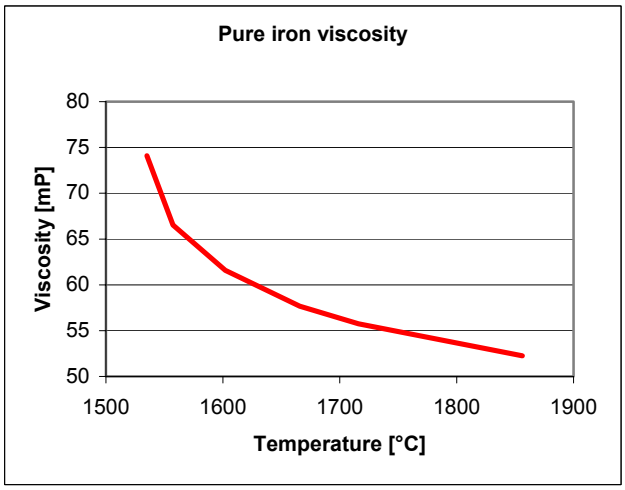


Specific heat vs. temperature diagram

- *Viscosity:*

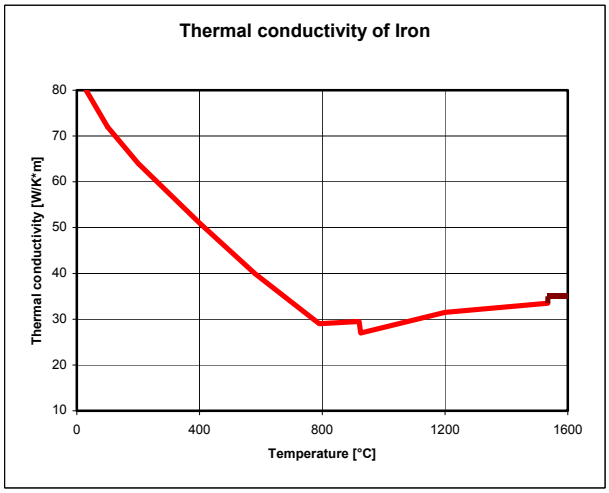
Temp [°K]	*v [kg/(m*s)]*
1808	0.0074087
1830.41	0.00665226
1875.11	0.00615849
1938.84	0.00576669
1988.97	0.00557522
2129.21	0.00522546

Viscosity vs. temperature diagram→



- *Thermal conductivity:*

Temp [°K]	*Tc[W/(m*K)]*
303	80
373	72
473	64
673	51
853	40
1063	29
1193	29.5
1198	27
1473	31.5
1808	33.5
1808.1	35
2273	35



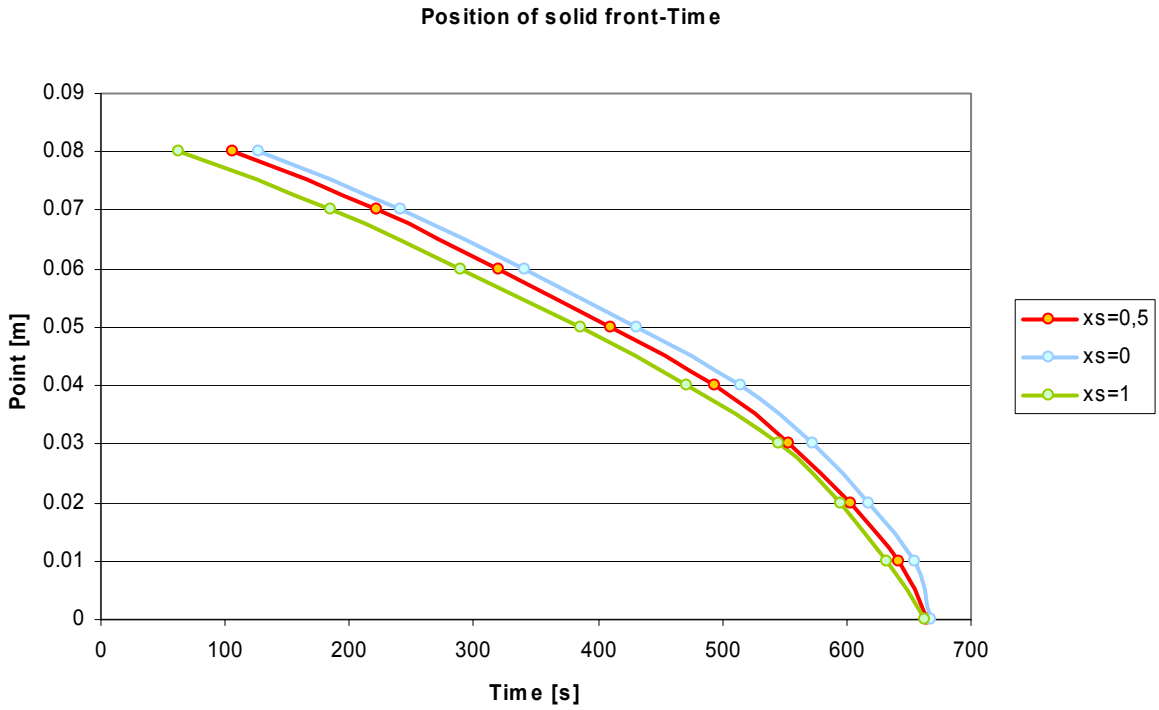
Thermal conductivity vs. temperature diagram

Another very important thing are the numerical parameters used to solve the simulation for Iron. The table below shows which ones I had used:

SOLVER CONTROLS					
Iter	Shared	Max. Iterations	*1000*		
		Convergence Crit.	*0.00001*		
		Min. Residual	*1E-18*		
Spatial	Spatial Differencing	Enthalpy	*Upwind*		
Solvers	Solvers	Enthalpy	*CGS+Pre*	*2500*	*0.00001*
Relax	Inertial Relaxation	Enthalpy	*0.5*		
	Linear Relaxation	Temperature	*0.2*		
Limits		Enthalpy	*-1E+20*	*1E+20*	
		Temperature	*1E-10*	*5000*	
Adv	Heat transfer	CFL Relaxation	*Disabled*		

For more information about the input numerical parameters, please look at *CFD-ACE(U) User Manual – Chapter 12: Numerical Parameters*.

After the simulation, I obtained the following results:

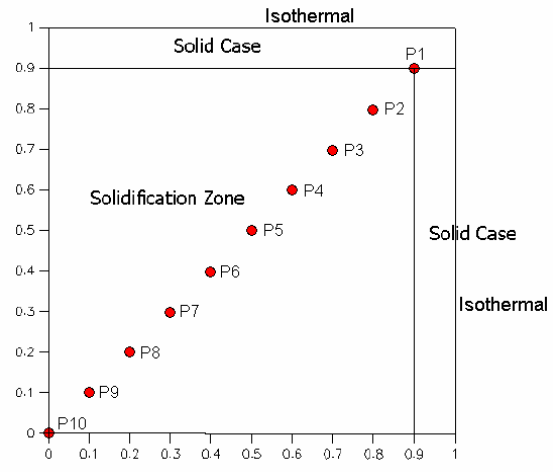


The way I had obtained this diagram and the conclusions of the simulation are explained below. (for more details and information about the diagram and the data, look at Q:\agspitz\cfdrc\Mia\Case\Iron+Aluminia crucible).

5 How were these diagrams obtained?

Using the CFD-VIEW program it's possible to get all the values and diagrams needed. Using the animation simulation tools and the plot function it's easier to see and understand the whole solidification process.

The diagrams are showing the position of the solid fraction front in each point of the box (see attached picture with the red spots) against time, so we can realize how fast solidifies the metal in each point of the solidification zone. x_s=1 means the metal have already solidified and x_s=0 it's when the metal starts to solidify. It's also a good reference to study when x_s=0.5.

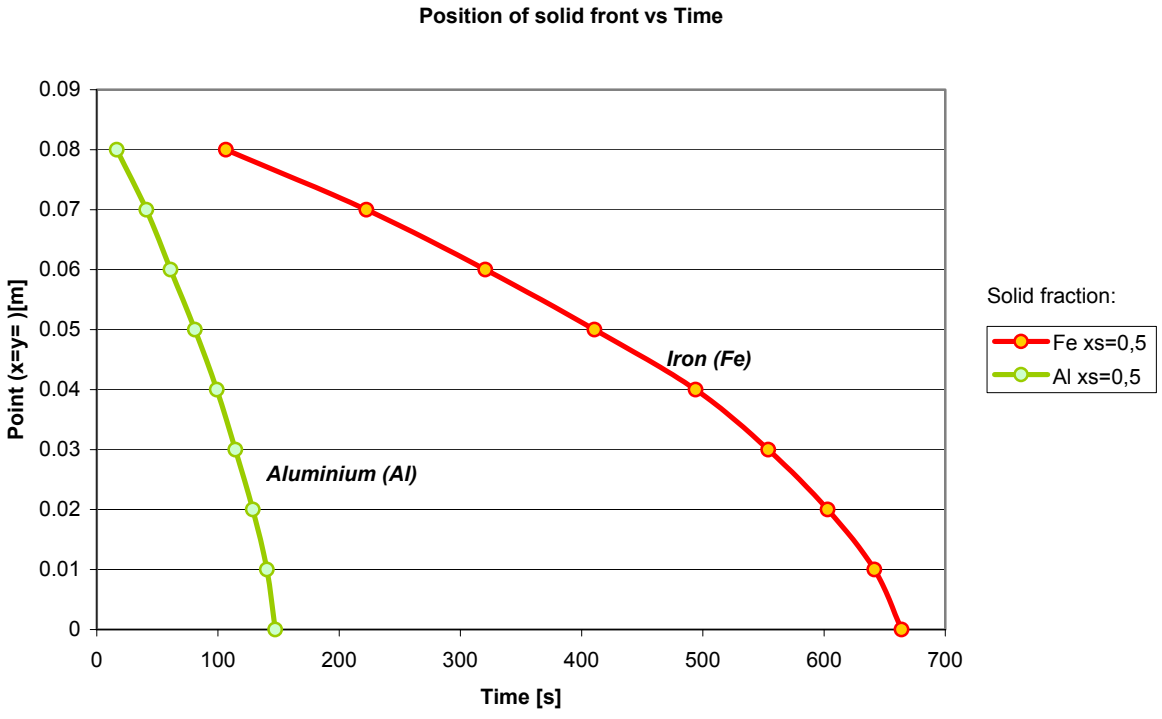


6 Summary and conclusions

The aim of this report is to compare the solidification process for Aluminium and Iron. Due to their different physical properties I had to describe a method which allows to compare the two metals so they have to carry out the same amount of energy by conduction. The equation used was the following: (I set the ΔT for Iron to 100°)

$$Q_{T_0 \to T_S}\Big|_{Fe} = Q_{T_0 \to T_S}\Big|_{Al}$$

The results are the diagrams above. In order to realize the differences, I also show the comparison between the two diagrams with a solid fraction of x_s=0,5:



We can realize that the box with iron needs more time to solidify due to its worse thermal conductivity and specific heat values. The values of thermal conductivity for iron are lower than Al values, so Fe can't conduct heat as well as Al. And also the value of latent heat for iron is higher so Fe contains more heat (Joules) per kg.

The sum of all these factors play against the speed of solidification of Iron, concluding that Al can carry out faster the overall energy to solidify by conduction.

7 References

- ***Handbook of Chemistry and Physics***, by Chemical Rubber Co. 50th Edition
- ***Physikalische Stoffeigenschaften der reinen Metalle***, VSI-Handbuch Betriebstechnik
- ***The Viscosity of Liquid Iron and Iron-Carbon Alloys***, by R. N. Barfield and J. A. Kitchener, published in **Journal of the Iron and Steel Institute**, August 1955.
- ***CFD-ACE(U) User Manual***, Version 2002 by CFD Research Corporation.
- ***CFD-ACE(U) Modules***, Version 2002 by CFD Research Corporation.