

Please create separate MATLAB scripts for each sub-question where appropriate, using the following naming convention: "Question1a.m", "Question1b.m", "Question1c.m", etc. If you create your own functions, include them within the submission. Note some scripts will be similar to previous scripts, with minor modifications to answer the next question.

The assignment questions are designed to increase in difficulty. You may wish to solve the first few parts of the question and then revisit the last questions once you are experienced in solving heat transfer and diffusion problems using finite difference, and coding in MATLAB.



## Problem 1: Homogenization times

The chemical segregation of Rhenium in a cast and extruded Nickel superalloy has been measured using wavelength dispersive spectroscopy (WDX). The diffusivity of Rhenium in the FCC austenite phase has a diffusivity coefficient of  $7.868 \times 10^{-6} \text{ m}^2/\text{s}$ , and an activation energy of 287.3 kJ/mol. A solid solution heat treatment is required to homogenize the dendritic segregation of Rhenium so that the difference between the maximum and minimum concentrations are less than 0.15 at%.

- a) How long is needed to homogenize the chemical segregation using the diffusion distance formula for a 3D problem and a grain size of  $12 \mu\text{m}$  and a temperature of  $1150^\circ\text{C}$ ? 🌶️ (2 marks)

A more accurate calculation of the homogenization process is required. This is to be achieved by modelling diffusion of the concentration field measured at the grain boundary. The concentration field is approximated by the following Gaussian waveform:

$$c(x, t = \tau) = c_0 + \frac{M}{(4\pi D\tau)^{1/2}} \exp\left(\frac{-x^2}{4D\tau}\right) \quad 1$$

$$M = c_s(4\pi D\tau)^{1/2} \quad 2$$

Where  $c_0$  is 1%,  $c_s$  is 5%,  $x$  is the distance from the grain boundary and  $\tau$  is 100s. The concentration profile is presented in Figure 1, showing different options of how to model the concentration profile at the grain boundary interface.

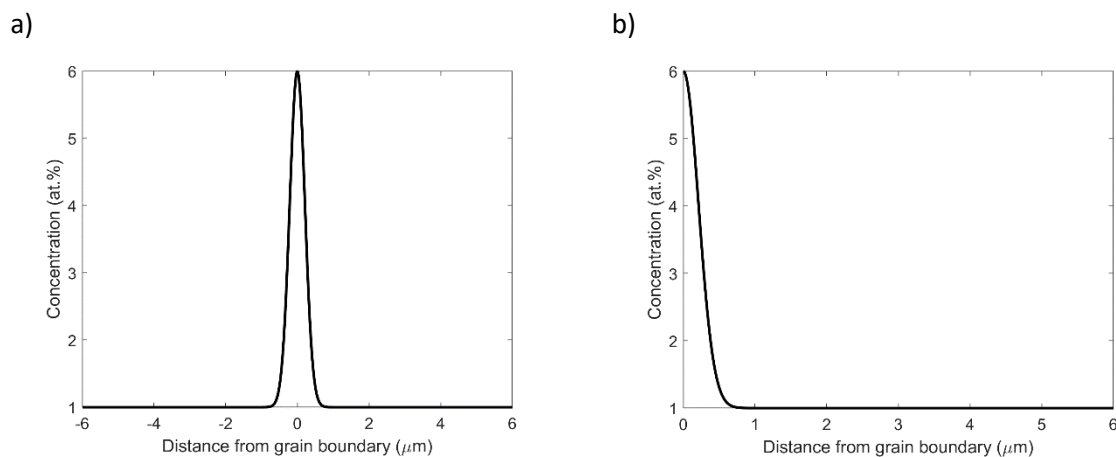



Figure 1: a) The initial concentration field of Nb considering plus or minus half a grain. b) The initial concentration gradient accounting for symmetry in the concentration profile.


- b) Write down a finite difference scheme for solving the diffusion equation in one dimension, using Ficks' first law of diffusion. Choose a representation of the concentration profile shown in Figure 1 and specify suitability boundary conditions. 🌶️ (4 marks)
- c) Implement the model and calculate the concentration field after 3h at  $1150^\circ\text{C}$ . Create a figure that compares your calculation to the analytical solution. 🌶️ (5 marks)
- d) How long is needed to reduce homogenize the segregation so that the difference between the maximum and minimum concentration is less than 0.15%? 🌶️ (3 marks)
- e) The diffusivity of Rhenium in FCC nickel has the following composition dependence.

$$D_v = D_0 \exp\left(-\frac{Q_0}{R_g T}\right) \quad 3$$

$$D_0 = 7.8682 \times 10^{-6} \times (1 + 9.9286 \times 10^{-4} X_{Re}) \quad 4$$

$$Q_0 = 287776.2 \times (1 - 0.1537924 X_{Re}) \quad 5$$

Where  $Q_0$  is the activation energy (J/mol) and  $D_0$  is the diffusivity coefficient ( $\text{m}^2/\text{s}$ ).  $R_g$  is the gas constant, and  $T$  is the absolute temperature. Note the composition in Equations 4 and 5 is in atomic fraction, not atomic percent. Present the finite difference scheme that includes a composition dependent diffusivity.  (4 marks)

- f) Quantify the impact of the composition dependent diffusivity upon predicting the required homogenization time.  (4 marks)

## Problem 2: 1D steady state temperature profiles in a pipe

The partial differential equation describing heat transfer in the radial direction of a cylinder is given in Equation 6.




$$\rho C_p \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left( r k \frac{\partial T}{\partial r} \right) = 0 \quad 6$$

If the inner and outer temperature are fixed and the thermal conductivity does not change with temperature, the analytical solution for steady state conditions where  $\frac{\partial T}{\partial t} \rightarrow 0$  is given by

$$T(r) = \frac{T_1 \ln\left(\frac{r_2}{r}\right) + T_2 \ln\left(\frac{r}{r_1}\right)}{\ln\left(\frac{r_2}{r_1}\right)} \quad 7$$

Where  $r$  is the position along the radius of interest,  $r_1$  is the inner diameter and  $r_2$  is the outer diameter.  $T_1$  and  $T_2$  are the temperatures at the inner and outer diameters of the cylinder. Please refer to Dr Travis' Lecture 5 for details about the derivation of this equation.

Model the 1D radial temperature profile within a stainless-steel pipe where the temperature at the inner radius is  $300^\circ\text{C}$  and at the outer radius it is  $180^\circ\text{C}$ . Assume a density of  $7850\text{kg}/\text{m}^3$ , a thermal conductivity of  $17\text{W}/\text{m}/\text{K}$ , and a specific heat of  $0.444\text{kJ}/\text{kg}/\text{K}$ . The inner radius is  $12.5\text{cm}$  and the pipe is  $3\text{cm}$  thick.

- Derive the finite difference scheme with and without temperature dependent thermophysical properties.  (7.5 marks)
- Create a labelled figure which compares the analytical and numerical solutions to this problem considering the case without temperature dependent properties.  (7.5 marks)
- The thermophysical properties of stainless steel are now considered temperature dependent. The temperature dependence of the thermal conductivity and specific heat are given in equations 8 and 9, given in units of  $\text{W}/\text{m}/\text{K}$  and  $\text{J}/\text{kg}/\text{K}$ , respectively. Create a labelled figure that compares the impact of the temperature dependent properties with the analytical solution. (Hint: an iterative approach is needed to approximate the temperature dependent thermal conductivity)  (7.5 marks)

$$k(T) = 14.52 + 0.128 T(^{\circ}\text{C}) \quad 8$$

$$C_p(T) = 414.7 + 0.155T(^{\circ}C)$$

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- d) What heat fluxes are required on the inner and outer radii to maintain this temperature profile with the original temperature independent thermal conductivity, and with the temperature dependent thermal conductivity? 🏹 (7.5 marks)

### Problem 3: Quench simulation

A series of experiments have been performed to characterize the water quench process of cylindrical pressure vessels. The quench tank has adjustable agitation. The experiments have measured the cooling rate of the cylinder at different locations across the radial direction for different agitation settings. The quench agitation can be set to a maximum setting of 10. The cylinders are placed vertically above the agitation propellers, achieving faster flow rates of water through the internal diameter of the workpiece in comparison to the outer surface. The component is heated to 900°C prior to the quench.

The quenched components are made out of the steel A508-3. The cylindrical geometry has an internal diameter of 2.5m and thickness of 0.225m. The thermocouple data can be downloaded from Blackboard for three experiments at different agitation levels. The location of the thermocouples is illustrated in Figure 2. The thermocouples are labeled "Ac1", "Ac2", and "Ac3".

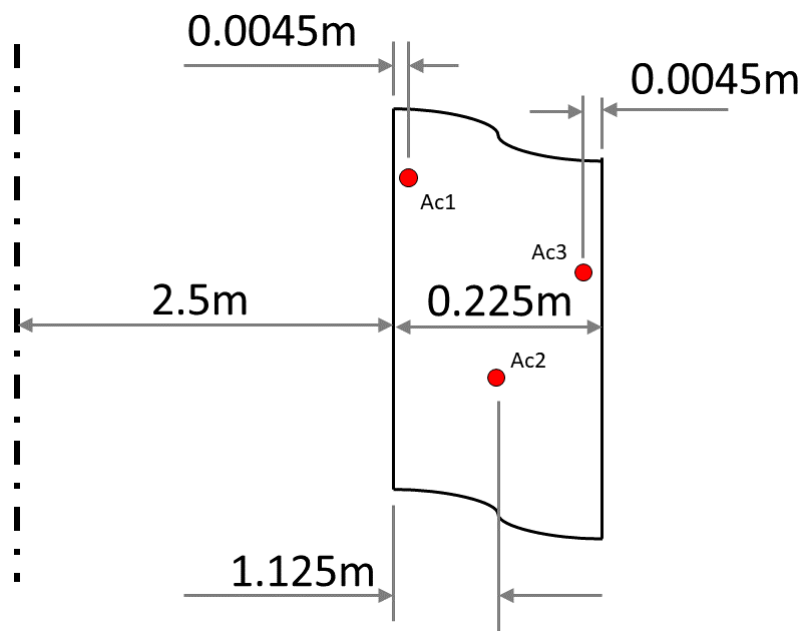


Figure 2: The geometry of the cylinder and location of the three thermocouples positioned close to the inner, middle, and outer diameter of the component.

The thermophysical properties of A508-3 are given in Equations 10 to 12. The emissivity is approximately 0.316. Note the temperature dependence of the thermal conductivity changes at 1066K and the temperature dependence is given in units of Kelvin.




$$\rho(T) = 7939.8 + 0.32912 T(K) \quad 10$$

$$\text{for } T \geq 1066K \quad k(T) = 14.6 + 0.01T(K) \quad 11$$

$$\text{for } T < 1066K \quad k(T) = 50.3 - 0.02T(K)$$

$$C_p(T) = 472.2 + 0.25 T(K)$$

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- a) Derive the finite difference schemes for a 1D heat transfer for the outer diameter, inner diameter, and for conduction inside the component. The partial differential equation for heat transfer through conduction considering cylindrical geometry is given in Equation 6. Consider radiative and convective heat losses, in addition to temperature dependent thermophysical properties.  (6 marks)
- b) Determine the heat transfer coefficients for the outer and inner diameter that best describes the datasets.  (8 marks)
- c) The heat treatments need to be designed to obtain predominately bainitic microstructures and reduce the amount of ferrite formed. To avoid excessive ferrite formation, a cooling rate greater than 0.28K/s is needed within the temperature window of 710°C to 570°C. What depth within the inner diameter meets this criteria for each condition?  (7.5 marks)