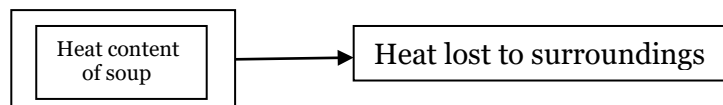
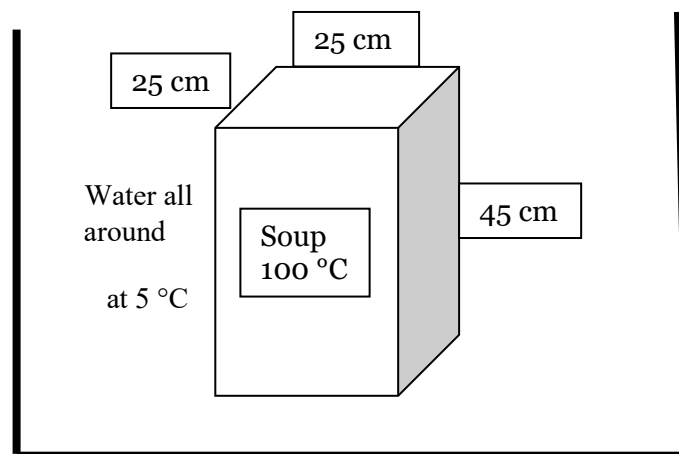

Modelización mediante ecuaciones diferenciales

Máster en Ingeniería Computacional y Matemáticas

1. We are going to cook a big pot of soup late at night and we know that refrigeration is essential to preserve the soup overnight. However, the soup is going to be too hot to be put directly into the fridge once it is going to be ready (the soup is going to be 100°C , and our fridge is not powerful enough to accommodate a big pot of soup if it is any warmer than 25°C). We're planning to cool the soup by first pouring it into a hermetic recipient and then immerse the hermetic recipient in a sink full of cold water, (kept running, so that its temperature is going to be roughly constant at 5 degrees). The recipient is a square prism whose width, depth and height are respectively 25cm, 25cm and 45 cm, and we know that the density of the soup is $\rho = 1.05 \text{ kg/l}$, the specific heat of soup is $c = 3000 \text{ J kg}^{-1} \text{ }^{\circ}\text{C}^{-1}$ and the heat transfer coefficient is $h = 24 \text{ W m}^{-2} \text{ }^{\circ}\text{C}^{-1}$.
- (a) Write the word equation and the differential equation that describes the problem. Explain the steps used to come to your answer.



Consideration: I will use the newton's law of cooling instead of the natural law of cooling because the water is running like if we have breeze.

Assumptions made:

1. First, let us assume that the soup in the container is well stirred so that the temperature remains homogeneous throughout.
2. We also assume that heat is lost from the surfaces of the container according to Newton's law of cooling
3. we assume that thermal constants, such as the specific heat and the Newton cooling coefficient, remain constant in our applications
4. The system has an infinite thermal conductivity. So that there is no variation of temperature inside the system,
5. The temperature is a function of time only
6. Total heat capacity is considered as one lumped and this analysis called as lumped heat capacity analysis /Newtonian heating (or) cooling process

The word equation is as follows:

$$(\text{rate of change of heat content}) = (\text{rate heat lost to surroundings})$$

The differential equation

$$m c \frac{dU}{dt} = -hS(U - u_s).$$

$m = \rho v$ (mass of the system)

u_s = value is constant

Using the newton cooling law

- (b) After keeping the recipient immersed in the sink of cold water for 30 minutes which will be the temperature of the soup?

Procedure

Separating the variables $\frac{dU}{(U-u_{s\infty})} = \frac{-hS}{cm} dt = \frac{-hS}{c\rho v} dt$

By Integrating the equation

$$\int \frac{dU}{(U-u_s)} = \frac{-hS}{cm} dt = \int \frac{-hS}{c\rho v} dt$$

$$\ln(U(t) - u_s) = \frac{-hS}{c\rho v} t + C_1$$

C_1 is the constant of Integration

The initial condition $U(0) = U_0$ and $t = 0$

Applying the above condition in equation, we get $C_1 = \ln(U_0 - u_s)$

Equation becomes

$$\frac{\ln(U - u_s)}{\ln(U_0 - u_s)} = \frac{-hS}{c\rho v} \cdot t$$

Equation to find out the temperature at a particular time instant.

$$\frac{U(t) - u_s}{U_0 - u_s} = \exp\left[\frac{-hS}{c\rho v} t\right]$$

Given data

$$u_s = 5^\circ \text{C}$$

$$m = 29.53$$

$$\rho = 1.05 \text{ kg/l} = 1050 \text{ kg/m}^3$$

$$c = 3000 \text{ J/kg}^\circ\text{C}$$

$$h = 24 \text{ W/m}^2\text{C}^1$$

$$U(30) \text{ in minutes} = ?$$

$$\text{Total surface Area (S)} = S_{\text{bottom}} + S_{\text{top}} + 4S_{\text{side}}$$

$$S_{\text{top}} = S_{\text{bottom}} = 0.25 \times 0.25 = 0.0625 \text{ m}^2$$

$$S_{\text{side}} = 0.25 \times 0.45 = 0.1125 \text{ m}^2$$

$$S = (2 \times 0.0625) + (4 \times 0.1125) = (0.125 + 0.45) \text{ m}^2 = 0.575 \text{ m}^2$$

If wall thermal resistance is negligible.

$$\text{Volume of Hermetic recipient (v)} = 0.25 \times 0.25 \times 0.45 \text{ m}^3 = 0.028125 \text{ m}^3$$

$$\frac{U_{30\text{min}} - 5}{100 - 5} = \exp\left[\frac{-24 \times 0.575 \times 30 \times 60}{1050 \times 3000 \times 0.028125}\right]$$

$$= \exp\left[\frac{-24840}{88593.75}\right]$$

$$U_{30 \text{ min s}} = 76.77^\circ \text{C}$$

- (c) How long should we keep the recipient immersed in the sink of cold water for the soup to reach a temperature of 24°C?

$$U(t) = 24^\circ\text{C}$$

$$t = ?$$

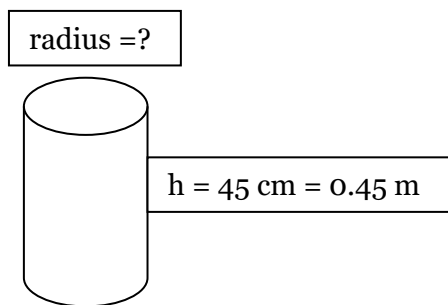
$$\ln \left[\frac{24-5}{100-5} \right] = \left[\frac{-24 \times 0.575}{1050 \times 3000 \times 0.028125} \right] t$$

$$-1.609 = \frac{-13.8}{88593.75} t$$

$$-1.609 = -0.000155t$$

$$t = 2.88 \text{ hours} = 173.0107 \text{ min}$$

- (d) If we use a cylindrical hermetic container of the same height and capacity would it be quicker or slower to cool the soup? Justify your answer.



$$\text{So } \pi r^2 L = 0.028125 \text{ m}^3$$

$$r^2 = \frac{0.028125}{3.14 \times 0.45}$$

$$\text{Radius of the container } r = 0.141 \text{ m}$$

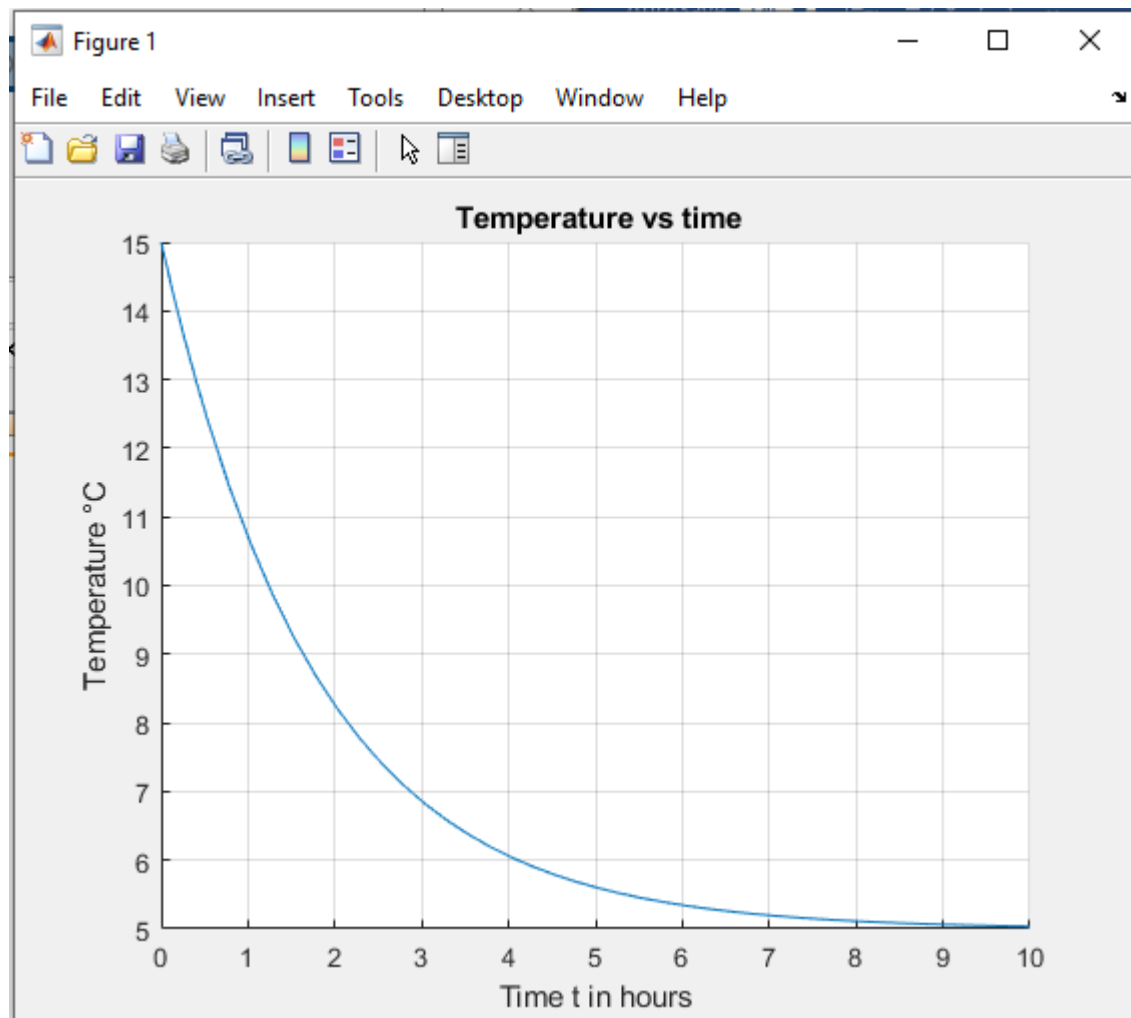
$$\text{Total surface area} = 2 \times \pi r^2 + 2\pi r L = 0.0398 + 0.3985 = 0.4383 \text{ m}^2$$

$$\ln \left[\frac{25-5}{95} \right] = \frac{-24 \times 0.4383}{88593.75} t$$

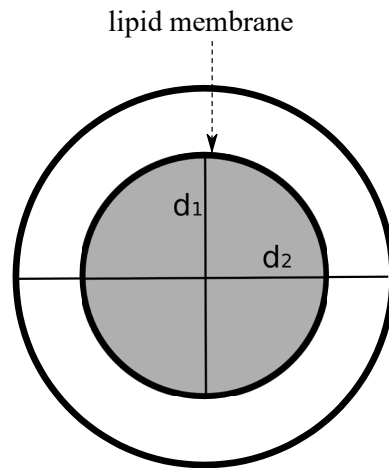
$$t = 3.6 \text{ hours or } 218.7 \text{ minutes}$$

Cooling the soup will be slower if we use cylindrical container of the same capacity
In this case we have less area in touch with the water

Plot of temperature against time with not heat source

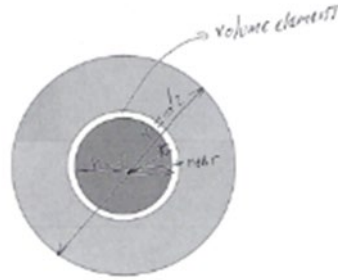


2. Liposomes are small spherical bilayer membranes that can be used to deliver drugs at a controlled rate. As they interact with the immune system they must be surrounded with an encapsulant material. The figure below represents this device. It is a spherical system where the liposome has diameter d_1 and is spherically encapsulated with a diameter d_2 . We assume that we have a drug inside the liposome that diffuses outwards in the radial direction.



- (a) Write down a suitable word equation for the rate of change of mass in a spherical shell r to $r + \Delta r$ and over a time interval t to $t + \Delta t$. Explain the steps used to come to your answer.

One-dimensional mass diffusion through a volume element in a sphere
 Let us consider a thin, spherical shell element of thickness Δr



Assumptions:

1. We assume that mass flows in the radial direction only; the mass inside the cylinder will then depend on r and the time t only.
2. If we also assume mass equilibrium, then the equilibrium mass will be a function of the radial distance r alone.



The rate of change for the mass of particles inside the region, is determined by the net amount flowing into and out of the region. Expressed as a word equation, this says that

$$\left\{ \begin{array}{l} \text{Rate of change of mass} \\ \text{in spherical shell} \end{array} \right\} = \left\{ \begin{array}{l} \text{rate of mass} \\ \text{conducted in at } r \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of mass} \\ \text{conducted out at } r + \Delta r \end{array} \right\}$$

- (b) Deduce a differential equation for the concentration at equilibrium. Explain the steps used to come to your answer.

A- Cross-sectional area normal to the mass flow

At equilibrium, the rate of change of mass with time will be zero, so the LHS is zero

The rate at which mass flows in at r is given by the mass flux (mass per unit time per unit area). Multiplied by the cross-sectional area, and similarly for the amount flowing out.

$$J(r)A - J(r + \Delta r)A = 0$$

Dividing by $A \Delta r$

$$(J(r + \Delta r) - J(r)) \div \Delta r = 0,$$

Taking the limit $\Delta r \rightarrow 0$

$$\frac{dJ}{dr} = 0 \quad \text{-----(1)}$$

Fick's Law of Diffusion

Fick's Law of diffusion describes the time course of the transfer of a solute between two compartments that are separated by a thin membrane, given by "<https://www.sciencedirect.com/>" and using substitution on (1)

$$\dot{J} = -DA \frac{dC}{dr}$$

D = diffusion coefficient

$$+ \frac{1}{A} \frac{d}{dr} \left(+DA \frac{dC}{dr} \right) = 0$$

Heat Transfer Area = $4\pi r^2$ = sphere area

$$+ \frac{1}{4\pi r^2} \frac{d}{dr} \left(+D4\pi r^2 \frac{dC}{dr} \right) = 0$$

For spherical geometries with radius r , where diffusion is towards the centre from the surface (or away from the centre towards the surface, If D is a constant then, the equation for equilibrium concentration with constant " D ", becomes

$$\frac{d}{dr} \left(r^2 D \frac{dC}{dr} \right) = 0$$

- (c) Now suppose that the diffusion coefficient depends on concentration instead of being constant. Does the differential equation in (b) remain the same? Justify your answer and write down the new equilibrium equation if it is the case.

Same procedure as about

$$\dot{J} = -D A \frac{dC}{dr}$$

D = diffusion coefficient

$$+ \frac{1}{A} \frac{d}{dr} \left(+DA \frac{dC}{dr} \right) = 0$$

Heat Transfer Area = $4\pi r^2$ = sphere area

$$+ \frac{1}{4\pi r^2} \frac{d}{dr} \left(+D4\pi r^2 \frac{dC}{dr} \right) = 0$$

This equation is for transient mass diffusion with variable diffusion coefficients (D).

$$+ \frac{1}{r^2} \frac{d}{dr} \left(+Dr^2 \frac{dC}{dr} \right) = 0$$

D = D(C)

This is the equilibrium concentration equation with variable “D”. So the differential equation for the concentration at equilibrium **is the same** as for differential equation when the diffusion coefficient depends on concentration instead of being constant.

And there is not mass source.

$$+ \frac{D}{r^2} \frac{d}{dr} \left(r^2 \frac{dC}{dr} \right) = 0$$

$$\frac{d}{dr} \left(r^2 \frac{dC}{dr} \right) = 0$$

3. Consider the equation for the scaled absolute temperature in an exothermic oxidation reaction with $\lambda = 2.2$,

$$\sigma \frac{d\theta}{dt} = 2.2e^{-1/\theta} - (\theta - \theta_a)$$

It's worth noting that the model assumptions listed in pag 262 of the textbook have been used.

- (a) For each of the three values $\theta_a = 0.11, 0.19$ and 0.27 generate a plot that allows you to determine the number of equilibrium solutions. Does the number of equilibrium solutions change with θ_a ? If the number of equilibrium solutions changes, interpret this change in terms of bifurcation theory.

$$\frac{d\theta}{dt} = 0 \text{ for equilibrium}$$

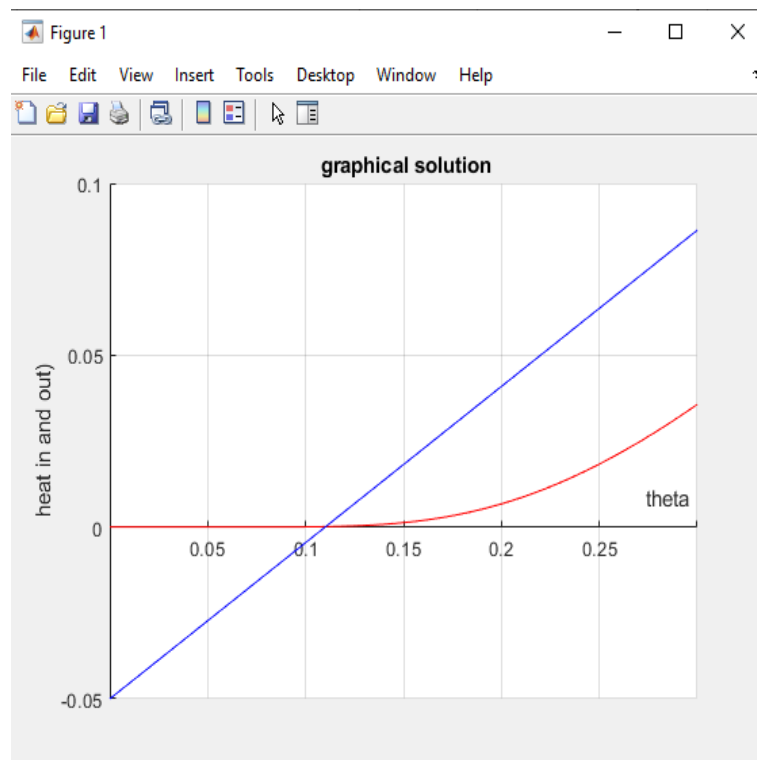
$$\lambda = 2.2$$

$$2.2e^{-1/\theta} = \theta - \theta_a$$

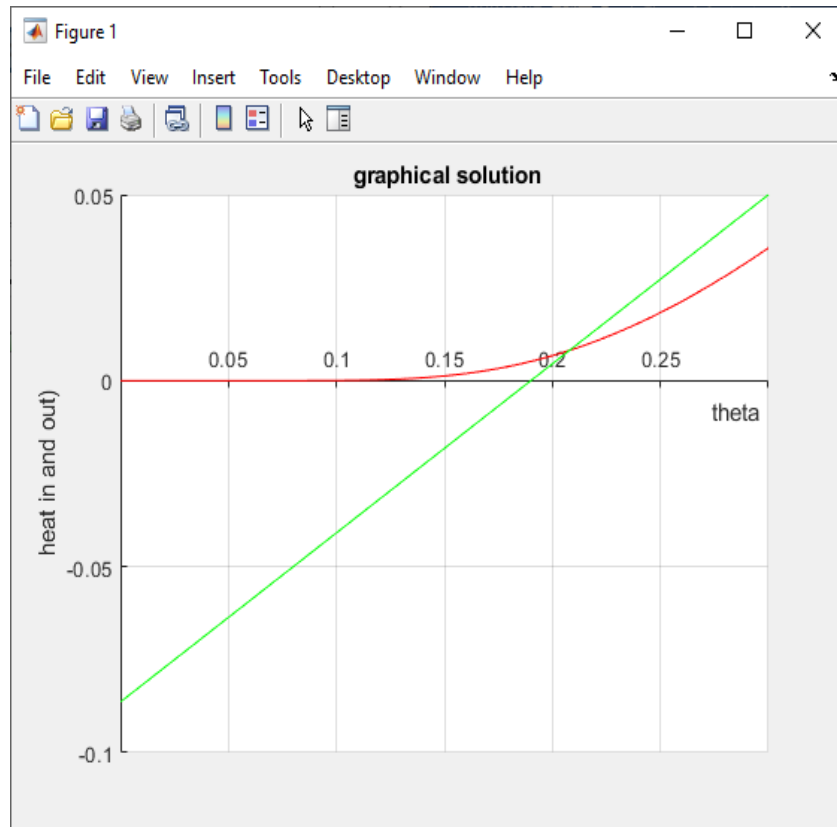
$$y = 2.2e^{-1/\theta}$$

$$y = \frac{1}{2.2}(\theta - \theta_a)$$

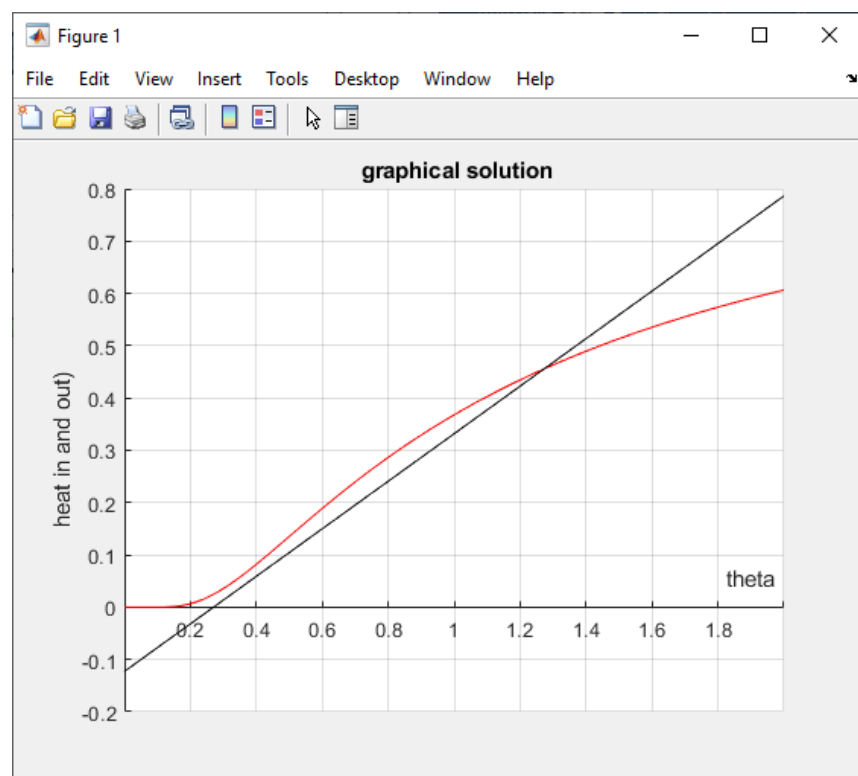
Plot for theta $\theta_a = 0.11$



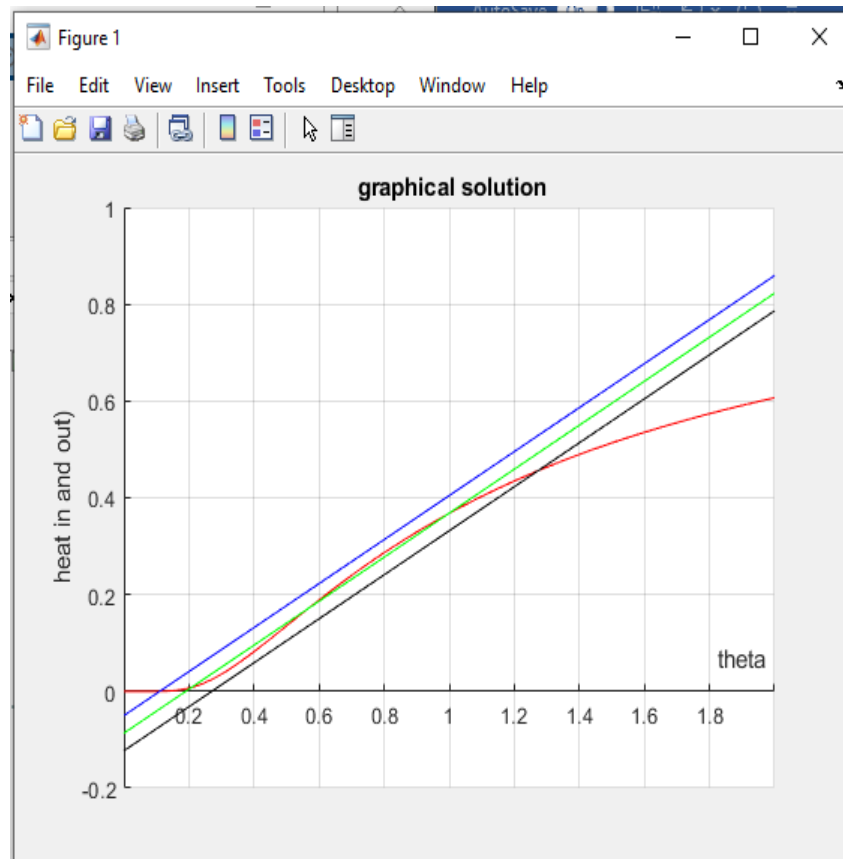
Plot for theta $\theta_\alpha = 0.19$



Plot for theta $\theta_\alpha = 0.27$

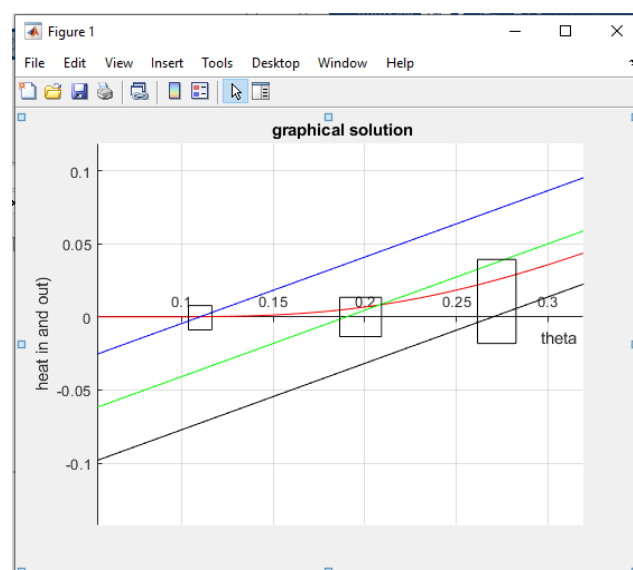


All of them



Yes the number of equilibrium solution change From the above plot we can see how the equilibrium solution change with the change of θ_α

As we increase θ_α we also move the slope of the line $(\theta - \theta_\alpha)$ and we reach critical values where the the number of equilibrium values change look like there is only one equilibrium value for $\theta_\alpha = 0.11$ there is only one solution , for $\theta_\alpha = 0.19$ we have three equilibrium values, and for



$\theta_\alpha = 0.27$ we have one equilibrium value the values of θ for which this changes occur are called bifurcation point.

(b) Show that if θ_{ac} is a critical ambient temperature where a bifurcation occurs then the equations

$$\theta_c^2 = 2.2e^{-1/\theta_c}, \quad \theta_{ac} = \theta_c - \theta_c^2$$

must be satisfied. In these equations θ_c is a critical scaled absolute temperature at which bifurcation occurs.

The occurrence of critical value temperature is written by

$$e^{-1/\theta_c} = \frac{1}{\lambda} * (\theta_c - \theta_a)$$

$$e^{-1/\theta_c} = \frac{\theta_c}{\lambda} - \frac{\theta_a}{\lambda}$$

given

$$\theta_c^2 = 2.2e^{-1/\theta_c}$$

From this we know that $\lambda = 2.2$

$$\lambda * e^{-1/\theta_c} = \theta_c - \theta_a$$

$$\lambda * e^{-1/\theta_c} - \theta_c = -\theta_a$$

$$\theta_c - \lambda * e^{-1/\theta_c} = \theta_a \quad \text{Where } \lambda = 2.2$$

If $\theta_c^2 = 2.2e^{-1/\theta_c}$ then by substitution in $\theta_c - \lambda * e^{-1/\theta_c} = \theta_{ac}$ we got

$$\theta_c - \theta_c^2 = \theta_{ac}$$

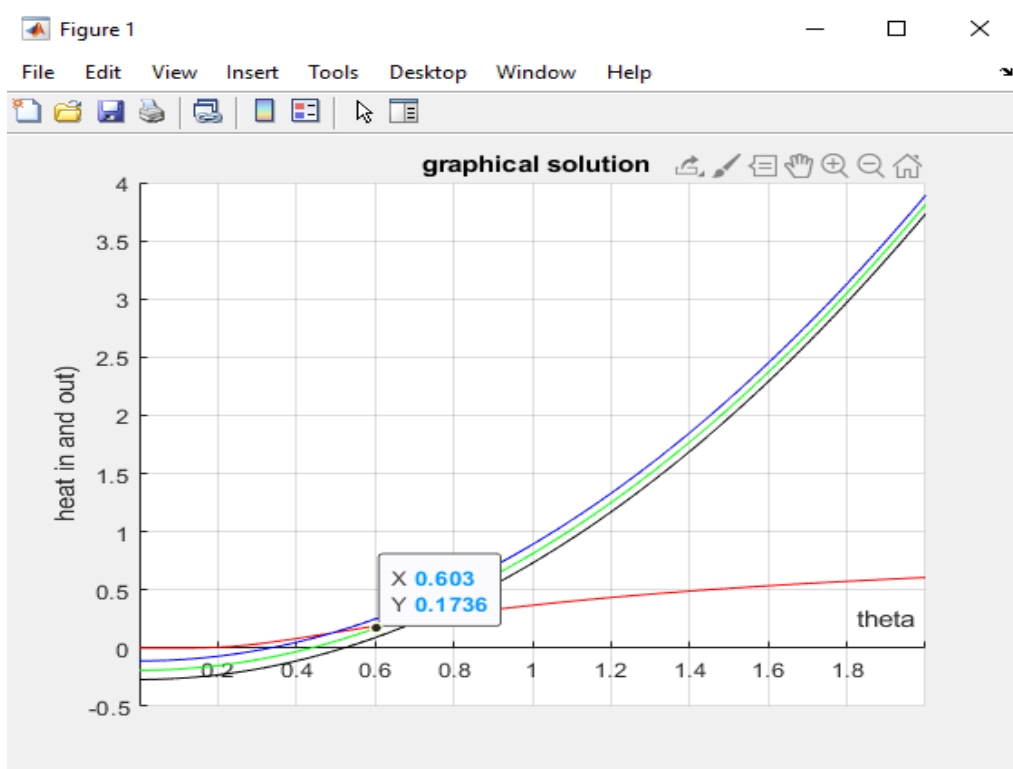
- (c) Use the equations in (b) to graphically estimate the critical ambient temperature θ_{ac} above which spontaneous ignition occurs. Give the numerical value of this estimation

$$\theta_c^2 = 2.2e^{-1/\theta_c}, \quad \theta_{ac} = \theta_c - \theta_c^2$$

$$\theta_c - \theta_c^2 = \theta_{ac}$$

$$\theta_c^2 - \theta_c + \theta_{ac} = 0$$

Using the same matlab program and plotting for different $\theta_a = 0.11, 0.19$ and 0.27 with $\lambda = \text{constant}$ you get the next plot



It is the second bifurcation in quadratic equation here that corresponds to thermal ignition, since, owing to the stability of the equilibrium points, the temperature to which the system evolves jumps suddenly from θ_1 to θ_3 . The value of θ_a where this occurs is the critical ambient temperature, θ_{ac} . This value is $\theta_{ac} = \pm 0.603$