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Introduction to Mathematical Modeling

In Affiliation With:

MBI
Microproducts Breakthrough Institute

PTT - LOA
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Mathematical Modeling

- Mathematical modeling is the process in which an appropriately complete understanding of a …

  physical-chemical-biological-sociological-physiological

  … "(sub) system" is converted into a set of mathematical expressions.
- These mathematical expressions constitute the mathematical model.
- In engineering we most often use conservation laws (first principles) as a basis for mathematical models.
- Mathematical models are useful for the prediction of *future states* of the system or the description of *current and past states* of the system.

Mathematical Modeling

What are the physical properties/quantities that are conserved and are subject of conservation laws?

mass

~~volume~~

energy

momentum

electron spin

Are there other physical quantities that could be a subject of conservation laws?

YES!

Are we interested in them within the framework of this course?

NO!

Mathematical Modeling

We are interested in modeling only: mass, energy, momentum, and chemical kinetics.

What is the simplest form of the conservation law that you have learned in previous courses?

Input - Output = Accumulation

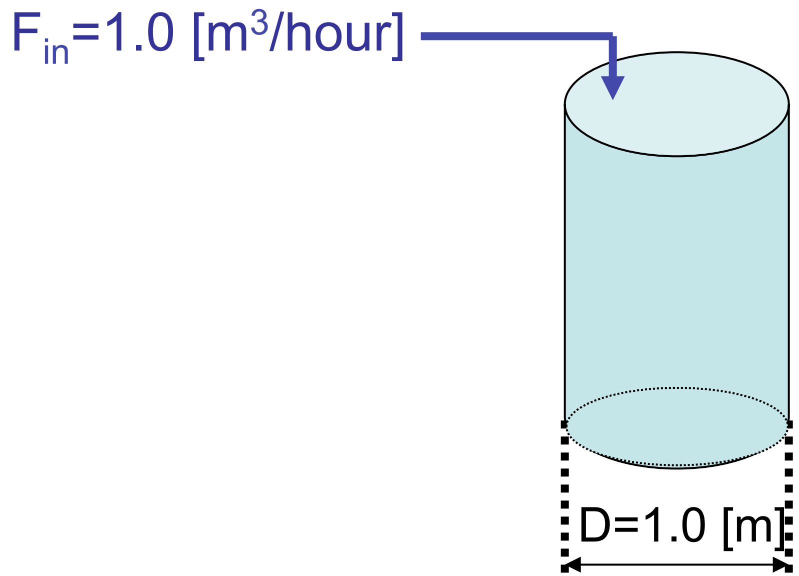
Both Input and Output are nominally positive quantities. The minus sign appearing in the above equation indicates that conserved quantity is “leaving” the system through the system boundary. It does not mean that the conserved quantity is negative by itself.

Mathematical Modeling

ACCUMULATION	=	Inventory of the system in **Position 2**	–	Inventory of the system in **Position 1**
ACCUMULATION	=	Inventory of the system at **Later Time**	–	Inventory of the system at **Earlier Time**

Mathematical Modeling

Let's consider a tank shown in illustration below, which is initially empty.



Question:

How is the level of the liquid in the tank changing with time?

Mathematical Modeling

Answer:

We will set up the mass balance of liquid in the tank.

<u>List of Variables:</u>

F_{in} (=) volumetric flow rate of liquid [m^3/hour]

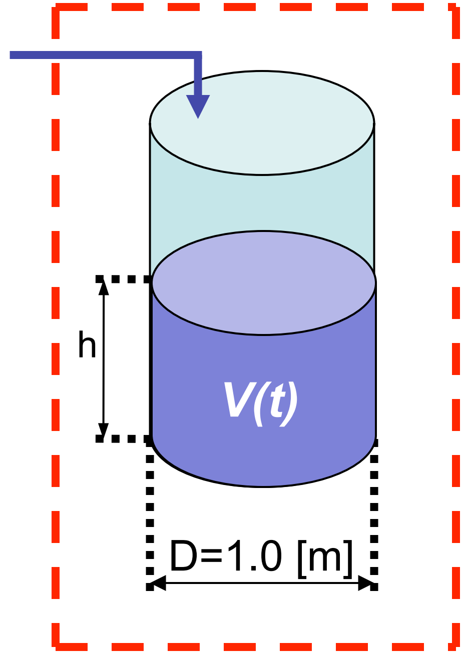
h (=) level of the liquid in the tank [m]

D (=) diameter of the tank [m]

ρ (=) density of the liquid [kg/m^3]

Next we will set the boundary of the system.

Mathematical Modeling



Apply the mass conservation law:

Input - Output = Accumulation [kg]

$$F_{in}\rho \cdot \Delta t \quad - \quad 0 \quad = \quad V\rho\big|_{t+\Delta t} \quad - \quad V\rho\big|_{t}$$

Mathematical Modeling

$$F_{in} \cdot \rho \cdot \Delta t = V \cdot \rho\Big|_{t=t+\Delta t} - V \cdot \rho\Big|_{t=t}$$

$$\left(\frac{\mathrm{m}^3}{\mathrm{s}}\right)\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)(\mathrm{s}) = \left(\mathrm{m}^3\right)\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$$

$$F_{in} \cdot \rho = \frac{V \cdot \rho\Big|_{t=t+\Delta t} - V \cdot \rho\Big|_{t=t}}{\Delta t}$$

$$\lim_{\Delta t \to 0}\left[F_{in} \cdot \rho\right] = \lim_{\Delta t \to 0}\left[\frac{V \cdot \rho\Big|_{t=t+\Delta t} - V \cdot \rho\Big|_{t=t}}{\Delta t}\right]$$

Mathematical Modeling

$$F_{in} \cdot \cancel{\rho} = \frac{d\left(V \cdot \rho\right)}{dt} = \cancel{\rho}\frac{dV}{dt} \quad \Rightarrow \quad F_{in} = \frac{dV}{dt}$$

… and if density is constant,

$$F_{in} = \frac{dV}{dt} \quad \rightarrow \quad F_{in} = \frac{d\left(\dfrac{\pi d^2 h}{4}\right)}{dt}$$

Mathematical Modeling

$$\rightarrow F_{in} = \frac{\pi D^2}{4}\frac{dh}{dt} \quad \rightarrow \quad \frac{dh}{dt} = \frac{4F_{in}}{\pi D^2}$$

$$\rightarrow dh = \frac{4F_{in}}{\pi D^2}\, dt \quad \rightarrow \quad \int dh = \frac{4F_{in}}{\pi D^2}\int dt$$

$$\rightarrow \int_{h=0}^{h=h} dh = \frac{4F_{in}}{\pi D^2}\int_{t=0}^{t=t} dt \quad \rightarrow \quad h = \frac{4F_{in}}{\pi D^2}\, t$$

Mathematical Modeling

The mathematical model in differential form is:

$$F_{in} = \frac{\pi D^2}{4} \frac{dh}{dt}$$

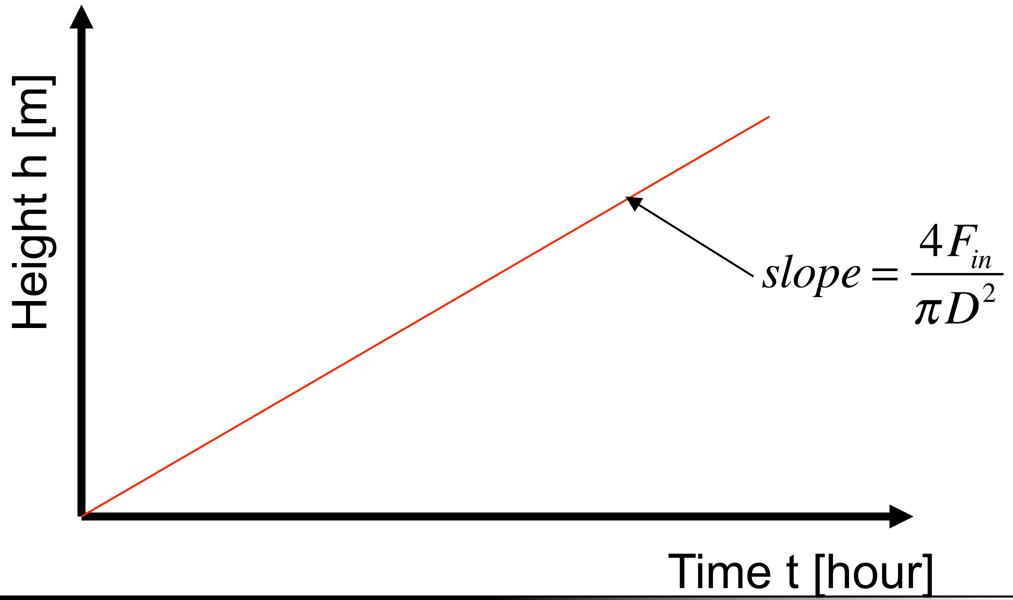
With the initial condition:

at $t=0$ $h=0$

Mathematical Modeling

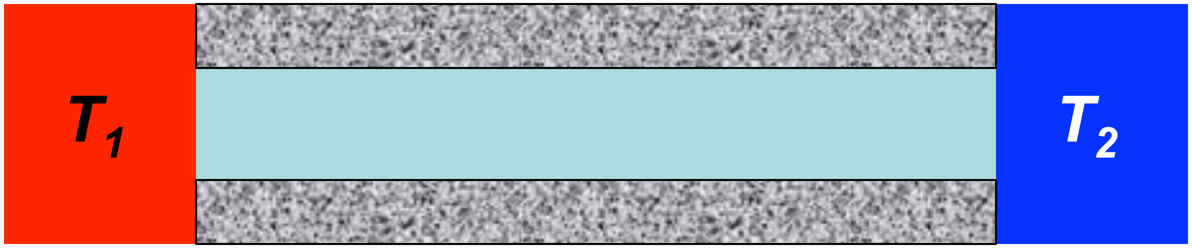
The mathematical model in integral form is:

$$h = \frac{4F_{in}}{\pi D^2}\, t$$

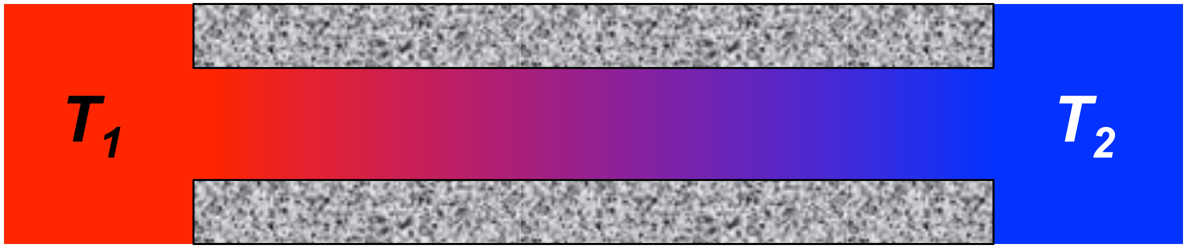


Mathematical Modeling

Let us now consider a metal bar positioned between two (large) heat sinks as shown in illustration below.



After reasonably long time, i.e. after a steady state conditions is reached, we may expect to find:



Mathematical Modeling

Question:

What is the temperature distribution in the metal rod at steady state?

Answer:

We will set up the energy balance (heat) in the rod.

List of Variables:

L (=) length of the rod [m]

k (=) thermal conductivity of the metal rod [J/mK]

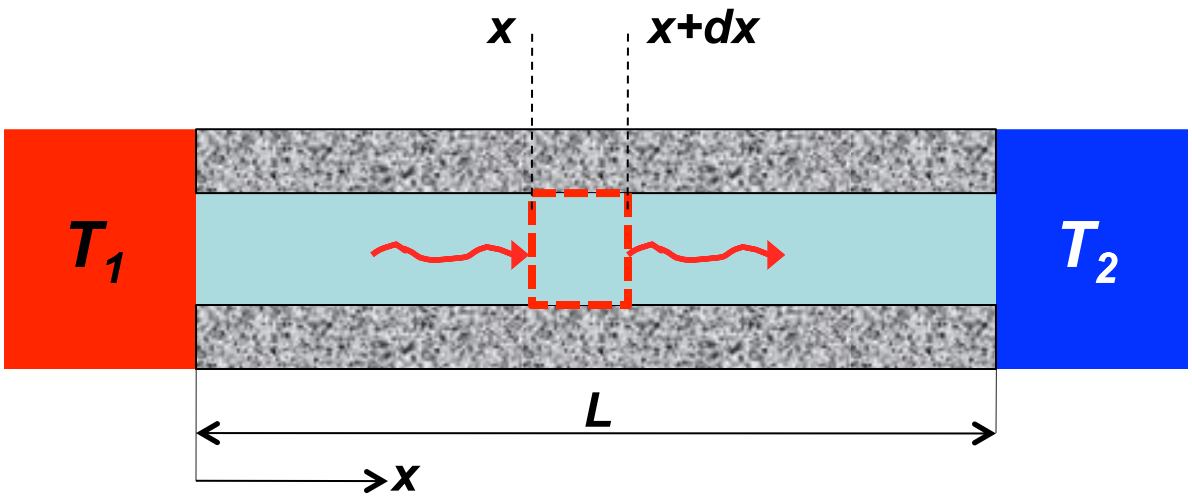
d (=) diameter of the rod [m]

ρ (=) density of the metal [kg/m^3]

C_p(=) specific heat of the metal rod [J/kgK]

Mathematical Modeling

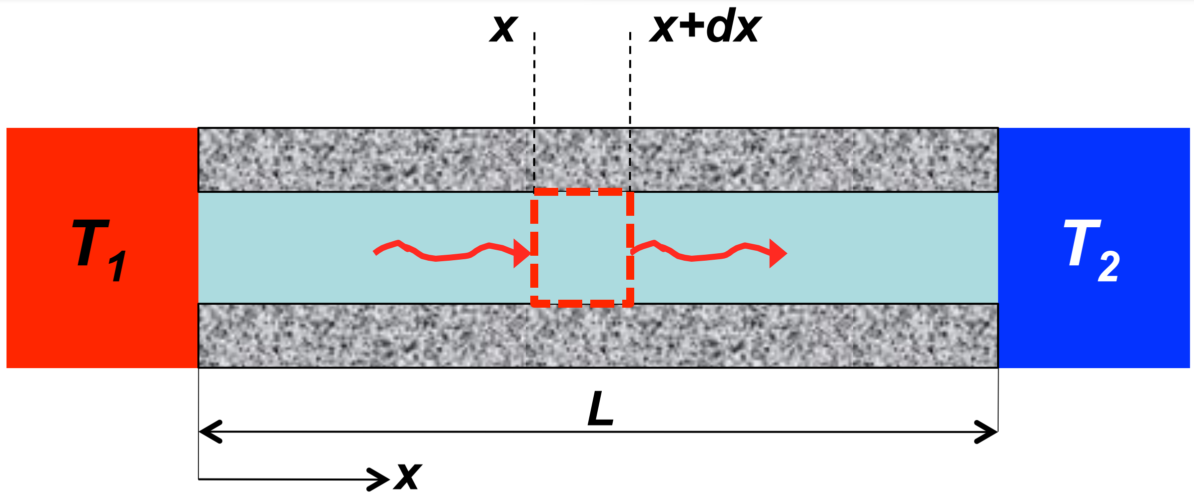
Since we are interested in the temperature distribution along the rod we will set up a differential energy balance across one differential element of at any non-specific position in the rod.



Apply the energy conservation law:

Input - Output = Accumulation [J]

Mathematical Modeling



Input - Output = Accumulation [J]

$$k\left(\frac{\pi d^2}{4}\right)\left(-\frac{dT}{dx}\right)\Bigg|_{x}\Delta t - k\left(\frac{\pi d^2}{4}\right)\left(-\frac{dT}{dx}\right)\Bigg|_{x+\Delta x}\Delta t = \rho C_p T\left(\frac{\pi d^2}{4}\right)\Delta x\Bigg|_{t+\Delta t} - \rho C_p T\left(\frac{\pi d^2}{4}\right)\Delta x\Bigg|_{t} \quad [J]$$

$$\left(\frac{J}{m\cdot K\cdot s}\right)\left(m^2\right)\left(\frac{K}{m}\right)(s) \qquad \left(\frac{kg}{m^3}\right)\left(\frac{J}{kg\cdot K}\right)(K)\left(m^2\right)(m)$$

Mathematical Modeling

$$k\cancel{\left(\frac{\pi d^2}{4}\right)}\left(-\frac{dT}{dx}\right)\Bigg|_{x}\Delta t - k\cancel{\left(\frac{\pi d^2}{4}\right)}\left(-\frac{dT}{dx}\right)\Bigg|_{x+\Delta x}\Delta t = \rho C_p T\cancel{\left(\frac{\pi d^2}{4}\right)}\Delta x\Bigg|_{t+\Delta t} - \rho C_p T\cancel{\left(\frac{\pi d^2}{4}\right)}\Delta x\Bigg|_{t}$$

$$k\left(\frac{dT}{dx}\right)\Bigg|_{x+\Delta x}\Delta t - k\left(\frac{dT}{dx}\right)\Bigg|_{x}\Delta t = \rho C_p T\Delta x\Big|_{t+\Delta t} - \rho C_p T\Delta x\Big|_{t} \qquad \text{Devide both side with } \rho C_p \Delta t \Delta x$$

$$\left(\frac{k}{\rho C_p}\right)\frac{\left(\frac{dT}{dx}\right)\Big|_{x+\Delta x} - \left(\frac{dT}{dx}\right)\Big|_{x}}{\Delta x} = \frac{T\big|_{t+\Delta t} - T\big|_{t}}{\Delta t}$$

$$\left(\frac{k}{\rho C_p}\right)\lim_{\Delta x\to 0}\left(\frac{\left(\frac{dT}{dx}\right)\Big|_{x+\Delta x} - \left(\frac{dT}{dx}\right)\Big|_{x}}{\Delta x}\right) = \lim_{\Delta t\to 0}\left(\frac{T\big|_{t+\Delta t} - T\big|_{t}}{\Delta t}\right) \quad \Rightarrow \quad \boxed{\left(\frac{k}{\rho C_p}\right)\frac{d^2T}{dx^2} = \frac{dT}{dt}}$$

Mathematical Modeling

At steady state: $\left(\frac{k}{\rho C_p}\right)\frac{d^2T}{dx^2} = \cancel{\frac{dT}{dt}} \Rightarrow \left(\frac{k}{\rho C_p}\right)\frac{d^2T}{dx^2} = 0 \Rightarrow \boxed{\frac{d^2T}{dx^2} = 0}$

Thus, mathematical model in differential form:

$$\boxed{\begin{array}{l} \qquad\qquad \dfrac{d^2T}{dx^2} = 0 \\ BC1: @ \quad x = 0 \quad T = T_1 \\ BC2: @ \quad x = L \quad T = T_2 \end{array}}$$

Now we can integrate (twice) the governing differential equation:

$$\frac{d^2T}{dx^2} = 0 \quad \Rightarrow \quad \frac{dT}{dx} = a \quad \Rightarrow \quad T = ax + b$$

Mathematical Modeling

Integration constants *a* and *b*, are determined from boundary conditions *BC1* and *BC2*;

$$T = ax + b \quad \Rightarrow \quad b = T_1 \quad \Rightarrow \quad a = \frac{T_2 - T_1}{L}$$

$$\boxed{\begin{array}{lll} BC1: @ & x = 0 & T = T_1 \\ BC2: @ & x = L & T = T_2 \end{array}}$$

Thus, the mathematical model in integral form:

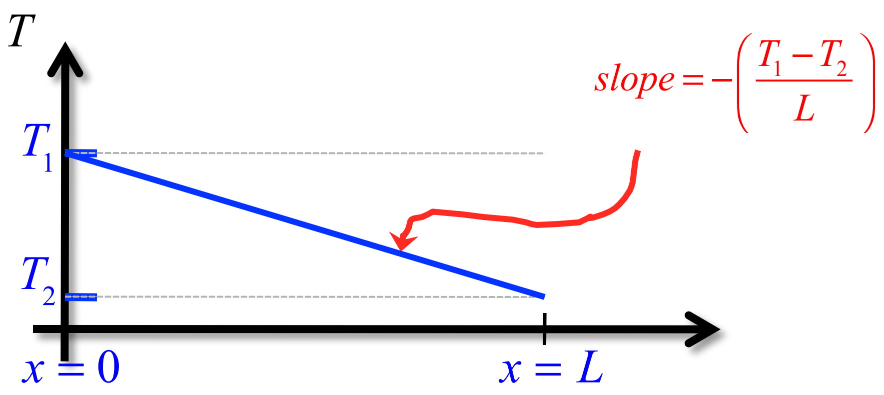
$$\boxed{T = -\left(\frac{T_1 - T_2}{L}\right)x + T_1}$$

Mathematical Modeling

Notice, that the form of the solution (for steady state condition) does not depend on physical properties (k, ρ, C_p) of the metal rod;

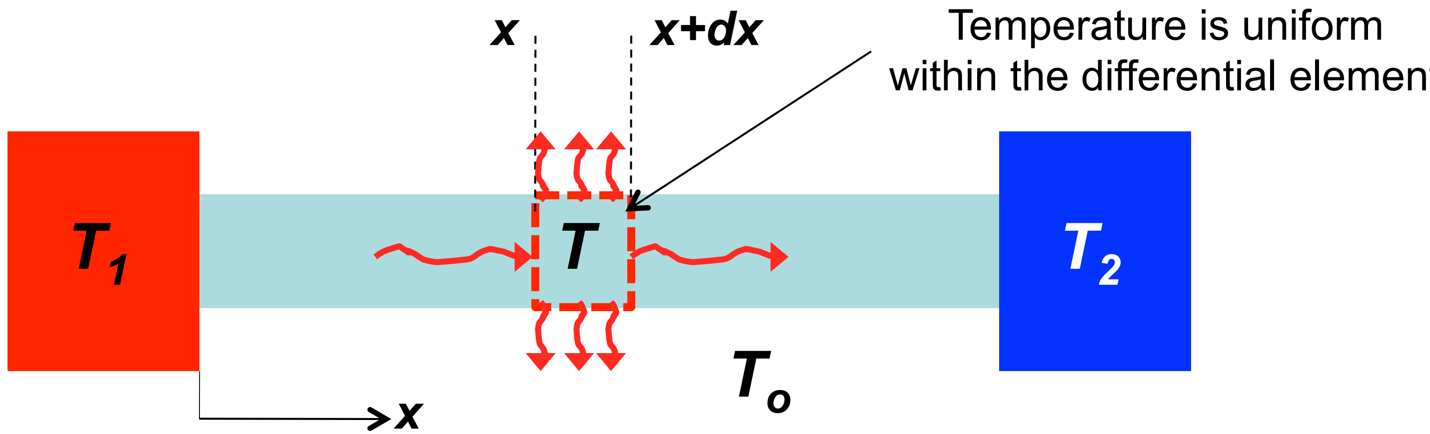
$$\boxed{T = -\left(\frac{T_1 - T_2}{L}\right)x + T_1}$$

And, the solution in graphical form;



Mathematical Modeling

Additional cases may be developed if physical situation changes. For example:



$$\left(\frac{k}{\rho C_p}\right)\frac{d^2T}{dx^2}-\left(\frac{4h}{\rho C_p d}\right)(T-T_o)=\frac{dT}{dt} \Rightarrow \boxed{\left(\frac{k}{\rho C_p}\right)\frac{d^2T^*}{dx^2}-\left(\frac{4h}{\rho C_p d}\right)(T^*)=\frac{dT^*}{dt}}$$

$$where \quad T^* = T - T_o$$

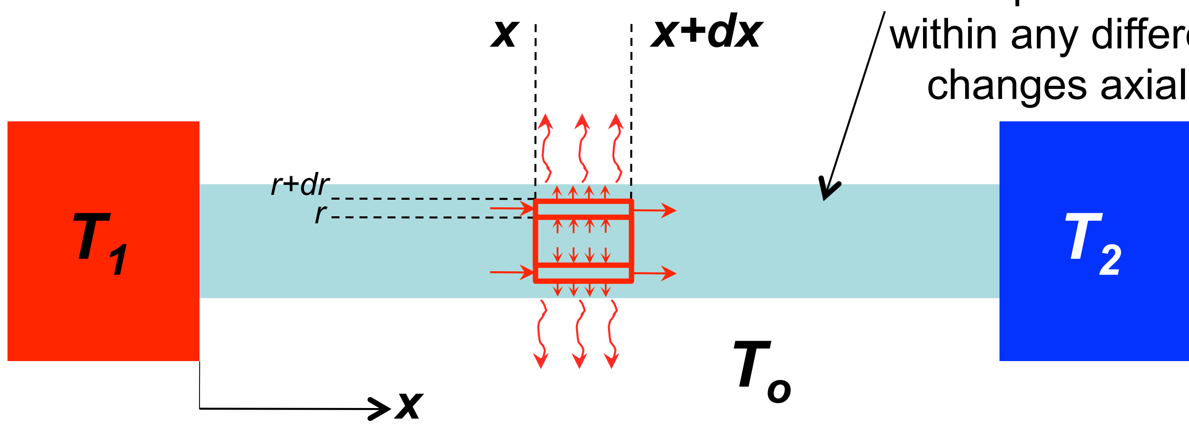
BC:

$$\boxed{\begin{array}{ll} @x=0 & T_{x=0}=T_1 \Rightarrow T^*_{x=0}=T_1-T_o \\ @x=L & T_{x=L}=T_2 \Rightarrow T^*_{x=L}=T_2-T_0 \\ @t=0 & T_{\forall x}=T_o \Rightarrow T^*_{\forall x}=0 \end{array}}$$

Mathematical Modeling

*Still, an additional case may be developed if temperature of differential element **is not** uniform.*

Temperature ***is not*** uniform within any differential element; it changes axially and radially.



$$\left(\frac{k}{\rho C_p}\right)\frac{d^2T}{dx^2}-\left(\frac{k}{\rho C_p}\right)\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)=\frac{dT}{dt} \Rightarrow \boxed{\left(\frac{k}{\rho C_p}\right)\frac{d^2T^*}{dx^2}-\left(\frac{k}{\rho C_p}\right)\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T^*}{\partial r}\right)=\frac{dT^*}{dt}}$$

$$where \quad T^*=T-T_o$$

BC:

$$@x=0 \quad T_{x=0}=T_1 \Rightarrow T^*_{x=0}=T_1-T_o \quad @r=0 \quad \left(\frac{\partial T^*}{\partial r}\right)=0$$

$$@x=L \quad T_{x=L}=T_2 \Rightarrow T^*_{x=L}=T_2-T_0 \quad @r=R \quad k\left(\frac{\partial T^*}{\partial r}\right)=h\left(T^*\right)_{r=R}$$

$$=T_o \Rightarrow T^*_{\forall x}=0$$

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People. Ideas. Innovation.

Thank you for your attention!