One dimensional steady state diffusion, with and without source. Effective transfer coefficients

21 mars 2017

For steady state situations ($\partial_t = 0$) and if convection is not present or negligible the transport equation reduces to Laplace's equation $\Delta H = 0$ or Poisson's equation $\Delta H = R_H$ if there is a source term. We consider here a few cases of one dimensional steady state diffusion and we also introduce the notions of heat transfer coefficient and thermal resistance.

1 Boundary conditions and transfer coefficients

1.1 Conditions on temperature, concentration and their gradients

At the interface between two materials, we need to specify the boundary conditions which will apply to the temperature and concentration fields. The temperature field has to be continuous at an interface, otherwise there would be a diverging temperature gradient, and according to Fourier's law, an infinite heat flux. If we use a continuum model of matter, an interface is a two dimensional object with zero volume and there cannot be a production or storage of heat at the interface. As a consequence, the heat flux normal to the interface should also be continuous.

Similar conditions apply for mass transport : mass cannot accumulate at an interface of negligible volume and the mass flux should be continuous across an interface. However, there are case that are quit specific to mass transport. Semi permeable membranes can restrict the motion of some chemical species and impose a discontinuity of concentration at an interface. Chemical reactions can take place at an interface, for example at the surface of a solid material acting as a catalyst. When a reaction takes place, the mass flux J_C will depend on the kinetics : $J_C = kC^m$ where m is the order of the reaction and k is a rate constant, usually varying with temperature $k \propto \exp(-E/k_B T)$, E being an activation energy. We will discuss in more detail these boundary conditions with chemical reactions when we analyze the design of a biochemical sensor.

1.2 Effective transfer coefficients at an interface

Aside from the continuity of temperature or concentration and their gradients, we can in many cases specify the value of temperature or concentration (Dirichlet boundary condition) or specify the value of the gradient of temperature or concentration (Neumann boundary condition). If transport occurs by diffusion only (i.e. when $Pe \ll 1$), the flux at an interface is simply given by the gradient of temperature or concentration multiplied by either the thermal conductivity or the mass diffusivity. However if the transport occurs by a combination of diffusion and convection ($Pe \geq 1$), the flux will depend in general of the velocity field and we will need a detailed analysis of the flow to compute it. Nevertheless, the convection diffusion equation is linear in temperature and concentration and this linearity implies that fluxes will vary linearly with the temperature and concentration differences imposed at the boundary of the system. This is why we can write in general the heat flux J_H or mass flux J_C at a boundary in the following manner :

$$J_H = h_H(T_1 - T_0) \text{ or } J_C = h_C(C_1 - C_0) \tag{1}$$

where T_1 (resp. C_1) and T_0 (resp. C_0) are the temperatures (resp. concentrations) on either side of the boundary and h_H (resp. h_C) is an effective heat transfer (resp. mass transfer) coefficient. The effective transfer coefficients are determined experimentally, but in some cases that we will discuss later in the course, they can be determined analytically. In the two problems considered below (heat flux through a composite wall and bioheat equation), we use these transfer coefficients to specify boundary conditions.

2 Planar geometry

If the geometry of the problem is such that gradients of temperature or concentration occur only in one directions (say x) in space, the transport equation in steady state is :

$$\frac{\partial^2 T}{\partial x^2} = 0 \qquad (2)$$

or

$$\frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}(x)}{\lambda} = 0 \qquad (3)$$

with a source term $\dot{q}(x)$ giving the amount heat produced par unit volume and per unit time. Here we consider specifically an heat transfer problem, since there are many examples in applications, but a steady state 1D mass transfer problem would be formally identical.

2.1 Thermal resistance

Without a source term, the solution of the equation has the general expression $T(x) = A + Bx$, A and B depending on the boundary conditions. The flux is given by : $J = -\lambda dT/dx = -\lambda A$ where λ is the thermal conductivity. If we consider now a material of thickness e in the x direction, the temperature gradient is $(T_1 - T_0)/e = \Delta T/e$ where T_1 and T_0 are the temperatures on the left and right sides of the material. Hence, the heat flux is $J = -\lambda \Delta T/e$. Using an analogy with Ohm's law for electrical conduction $I = U/R$, the heat flux being analogous to the current and the temperature difference to the electrical potential, we define a thermal resistance :

$$R_T = \frac{e}{\lambda}. \qquad (4)$$

2.2 Heat transfer through a composite planar structure

The notion of thermal resistance can be applied readily to composite planar systems such as a wall made of three different layers (fig. 1). There is a plaster layer of thickness e_p =1cm, with thermal conductivity $\lambda_p = 0.2$ W/m.K, a layer of glass fiber (e_f =10cm, $\lambda_f = 0.04$ W/m.K) and an outside layer of wood ((e_w =2cm, $\lambda_f = 0.12$ W/m.K). The air inside the house is at temperature T_i=20°C and the air outside at T_o=-5°C. We want to compute the heat flux J through the wall to estimate the power needed to keep the inside air at 20°C.

The heat flux is constant through the wall and is given by :

$$J = \frac{(T_1 - T_2)\lambda_p}{e_p} = \frac{(T_2 - T_3)\lambda_f}{e_f} = \frac{(T_3 - T_4)\lambda_w}{e_w}$$

T_1, T_2, T_3 and T_4 being the temperatures at the different interfaces from left to right.

We have for the temperatures :

$$T_1 = T_2 + \frac{Je_p}{\lambda_p} \text{ and } T_2 = T_3 + \frac{Je_f}{\lambda_f} \text{ and } T_3 = T_4 + \frac{Je_w}{\lambda_w}$$

and the total temperature difference is :

$$T_1 - T_4 = J\left(\frac{e_p}{\lambda_p} + \frac{e_f}{\lambda_f} + \frac{e_w}{\lambda_w}\right)$$

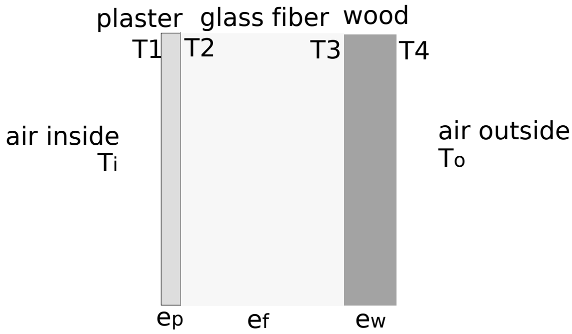

FIGURE 1 – A composite wall

The system is analogous to three resistors in series, we sum the individual thermal resistances to get the global resistance. If we examine the different resistances, we see that λ_f is an order of magnitude smaller than λ_p and λ_w. In addition, e_f is an order of magnitude larger than e_p and e_w. So we can consider that the thermal resistance of the wall is dominated by the layer of glass fiber and make the assumption :

$$T_1 - T_4 \approx J \frac{e_f}{\lambda_f}.$$

To close the problem, we need to write the boundary conditions inside and outside the house. The heat transfer at the inside and outside interfaces is dominated by convection and we use heat transfer coefficients determined experimentally, namely h_i=30 W/m^2.K and h_o=60 W/m^2.K. So, using these heat transfer coefficients, the heat flux is given by :

$$J = (T_i - T_1)h_i = (T_4 - T_o)h_o.$$

Then :

$$T_1 = T_i - \frac{J}{h_i} \text{ and } T_4 = T_o + \frac{J}{h_o}.$$

Finally :

$$T_1 - T_4 = T_i - T_o - J\left(\frac{1}{h_i} + \frac{1}{h_o}\right) = J\frac{e_f}{\lambda_f}.$$

and the value of the heat flux is given by :

$$J = (T_i - T_o)\left(\frac{1}{\frac{1}{h_i} + \frac{1}{h_o} + \frac{e_f}{\lambda_f}}\right)$$

Again, if we examine the values of the different terms, we can see that the dominant one is the thermal resistance of the glass fiber and we have : $J \approx (T_i - T_o)\lambda_f / e_f = 10$ W/m^2.

3 Cylindrical geometry

In a cylindrical geometry, where the temperature depends only on the radius r, the transport equation is in steady state :

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dT}{dr}\right) = 0 \tag{5}$$

Integrating twice, we the general solution : $T(r) = A\ln r + B$ where A and B are determined by the boundary conditions.

3.1 Uniform heat source

With a source term, the equation is :

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dT}{dr}\right)+\frac{\dot{q}(r)}{\lambda}=0 \tag{6}$$

If the production of heat is uniform in space, the integration with respect to r gives the general solution :

$$T(r)=-\frac{\dot{q}r^2}{4\lambda}+A\ln r+B \tag{7}$$

If we consider the case of a cylindrical metal wire with radius R in which an electric current generates heat by Joule effect at a rate $\dot{q}$, we can determine the temperature distribution within the wire from eqn. 7 by noting that T cannot diverge at the center of wire ($r=0$), hence $A=0$, and by specifying the surface temperature at R.

If we prescribe the surface temperature T_s, we have : $T_s=-\dot{q}R^2/4\lambda+B$ and :

$$T(r)-T_s=\frac{\dot{q}(R^2-r^2)}{4\lambda}. \tag{8}$$

The temperature distribution within the wire is parabolic with a maximum on the axis $T_m=T_s+\dot{q}R^2/4\lambda$.

3.2 Distributed heat source. The bioheat equation.

Mammals need to regulate precisely their internal temperature. This regulation is achieved by several mechanisms, one of which being the transport of heat by blood from the core of the body to the tissues in the limbs.

H. Pennes performed in 1948 a pioneering work in this domain by performing temperature measurements within forearms of human subjects (fig. 2) and developing a simple heat transfer model : the *bioheat equation*. In this model, the forearm is approximated as a cylinder made of a uniform muscle tissue and the temperature is assumed to depend only on the radial coordinate r. Heat is generated within the muscles by metabolic activity at a constant rate $\dot{q_m}$. In addition there is a heat transfer from the blood to the surrounding tissue at a rate $\dot{q_b}$ proportional to the difference of temperature between the arterial flow T_a and the local temperature $T(r)$, to the mass flow rate of blood per unit volume of tissue $\rho_b V_b$ and to the specific heat per unit mass of blood C_b, i.e. $\dot{q_b}=(T_a-T(r))\rho_b C_b V_b$. Putting these two heat sources in the transport equation 6 gives the bioheat equation in cylindrical coordinates :

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dT}{dr}\right)+\frac{\dot{q_m}+(T_a-T(r))\rho_b C_b V_b}{\lambda}=0 \tag{9}$$

The bioheat equation can be rewritten as :

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dT}{dr}\right)-\frac{\rho_b C_b V_b}{\lambda}\left(T(r)-T_a-\frac{\dot{q_m}}{\rho_b C_b V_b}\right)=0 \tag{10}$$

or :

$$r^2\frac{d^2\theta}{dr^2}+r\frac{d\theta}{dr}-Kr^2\theta=0 \tag{11}$$

where $\theta=T(r)-T_a-\dot{q_m}/(\rho_b C_b V_b)$ and $K=\rho_b C_b V_b/\lambda$. This last equation is a modified Bessel equation, with a solution of the form $\theta=AI_0(r\sqrt{K})$ where I_0 is the modified Bessel function of the first kind with zeroth order. The temperature at the surface of the limb ($r=R$) is $T_s=T_a+\dot{q_m}/(\rho_b C_b V_b)+AI_0(R\sqrt{K})$. We assume now that the heat flux on the skin is given by a heat transfer coefficient h_s, we have the following boundary condition :

$$-\lambda\left(\frac{dT}{dr}\right)_{r=R}=h_s(T_s-T_0) \tag{12}$$

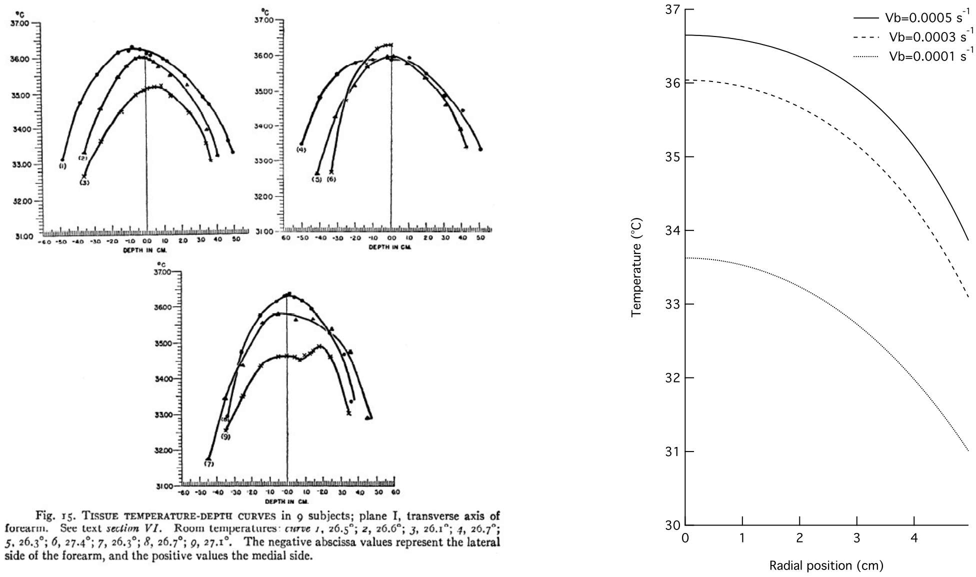

FIGURE 2 – Temperature profiles though a human forearm. Left, experimental results from H. Pennes, Journal of Applied Physiology, 1, 93 (1948). Different curves correspond to different room temperatures. Right, solutions of the bioheat equation for a cylinder of radius 5 cm, an outside temperature of 25°C and three different values of the blood flow rate.

where T_0 is the temperature of the ambient air. Using the relation for the Bessel functions : $dI_0(r)/dr = I_1(r)$, the boundary condition gives :

$$-\lambda A\sqrt{K}I_1(R\sqrt{K}) = h_s[T_a - T_0 + \dot{q_m}/(\rho_b C_b V_b) + AI_0(R\sqrt{K})] \tag{13}$$

yielding the integration constant :

$$A = -\frac{h_s[T_a - T_0 + \dot{q_m}/(\rho_b C_b V_b)]}{\lambda\sqrt{K}I_1(R\sqrt{K}) + h_s I_0(R\sqrt{K})} \tag{14}$$

The temperature distribution is finally given by :

$$T(r) = T_a + \frac{\dot{q_m}}{\rho_b C_b V_b} - \frac{h_s I_0(r\sqrt{K})[T_a - T_0 + \dot{q_m}/(\rho_b C_b V_b)]}{\lambda\sqrt{K}I_1(R\sqrt{K}) + h_s I_0(R\sqrt{K})} \tag{15}$$

or

$$\theta(r) = \frac{h_s I_0(r\sqrt{K})\theta_0}{\lambda\sqrt{K}I_1(R\sqrt{K}) + h_s I_0(R\sqrt{K})} \tag{16}$$

and the skin temperature is given by :

$$\theta_s = \theta(R) = \frac{\theta_0}{1 + \frac{\lambda\sqrt{K}I_1(R\sqrt{K})}{h_s I_0(R\sqrt{K})}} \tag{17}$$

There are two dimensionless parameters involved in this result : $R\sqrt{K}$ and $\lambda\sqrt{K}/h_s$. From a dimensional analysis of eqn. 9, we can see that $1/\sqrt{K}$ is a length scale such that the diffusive flux balances the flux due to the blood flow. If $R\sqrt{K}$ is small, this means that the radius R of the limb is small compared to $1/\sqrt{K}$ and we expect that losses by diffusion will be large and the heat convected by the blood flow will not be sufficient to maintain the skin temperature at a high enough value (say to prevent the skin from freezing).

The other dimensionless parameter $\lambda\sqrt{K}/h_s$ compare the heat flux generated by the blood flow and the heat flux due to the transfer to the surrounding air. If h_s gets very large, $\lambda\sqrt{K}/h_s$ goes to zero and the skin temperature goes down to the temperature of the surrounding air.

The typical value of the parameters are the following :

— thermal conductivity of muscles : $\lambda = 0.5$ W/m.K

— metabolic heat rate production $\dot{q_m} = 700$ W/m^3

— blood density $\rho_b = 1000$ kg/m^3

— blood specific heat $C_b = 3600$ J/kg.K

— blood flow rate per unit volume $V_b = 5 \times 10^{-4}$ s^{-1}

— heat transfer coefficient h_s=2 W/m^2.K

From these values we get $1/\sqrt{K} \approx 1.7$ cm and $\lambda\sqrt{K}/h_s \approx 1$. The temperature profiles within a limb of radius 5 cm (corresponding to a forearm), given by eqn. 15 are shown on fig. 2 for three different values of the blood flow rate. The curve with $V_b = 3 \times 10^{-4}$ s^{-1} reproduces rather accurately the experimental data recorded by Pennes.

4 Summary

— boundary conditions at an interface : continuity of temperature and heat fluxes. For mass transport, chemical reactions specify the mass flux through the kinetics of the reaction

— when convective transport is present, the flux at an interface can be modeled by an *effective transport coefficient*

— in a steady state one dimensional or axisymmetric heat transfer problems, we can define *thermal resistances* for materials and use analogies with electrical resistance networks to analyze the heat transfer characteristics of composite systems

— the formalism of heat transfer by diffusion, with internal production of heat, can be used to derive a *bioheat equation* modeling heat transfer through living tisues