Chapter 5

Formulation of FEM for Unsteady Problems

Two alternatives for formulating time dependent problems are called coupled space-time formulation and semi-discrete formulation. The first one treats the time similar to the space dimensions and make use of elements that have time dimensions. In this way the formulation of a 1D unsteady problem becomes very similar to that of a 2D steady problem. In coupled space-time formulation shape functions are considered to be functions of both space and time, and the approximate solution over an element for a 1D problem can be written as

$$u^e = \sum_{j=1}^{NEN} u_j S_j(x,t) \tag{5.1}$$

where NEN includes the element nodes in both space and time domains. Although coupled space-time formulation is very simple, it becomes computationally very expensive, especially for large 3D problems. Due to its efficiency, the second alternative, semi-discrete formulation became the standard way of studying time dependent problems.

In semi-discrete formulation time and space derivatives are discretized separately. Shape functions are taken to be functions of space only and discretization of space derivatives provide a set of ODEs involving time derivatives of the nodal unknowns. These ODEs are then discretized and solved using well-known ODE solution techniques.

5.1 Semi-Discrete Formulation – Space Discretization

To demonstrate how semi-discrete formulation works we'll use the following 1D, unsteady AD equation

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} - k\frac{\partial^2 T}{\partial x^2} = f \qquad \text{in} \quad \Omega \tag{5.2}$$

The scalar unknown T is a function of both space (x) and time (t). Together with two boundary conditions, we also need an initial condition (IC) that provides the solution on the whole domain at an initial time.

Weak form of this DE is obtained in the same way as we did for steady problems. First the weighted residual statement is written, followed by integration by parts applied to the diffusion term to yield the following elemental weak form

$$\int_{\Omega^e} \left(w\frac{\partial T}{\partial t} + wu\frac{\partial T}{\partial x} + k\frac{\partial w}{\partial x}\frac{\partial T}{\partial x} \right) dx = \int_{\Omega^e} wf\, dx \; + \; \text{B.T.} \tag{5.3}$$

where B.T. represents the boundary integral term. Approximate solution that we seek over an element is in the following form

$$T^e(x,t) = \sum_{j=1}^{NEN} T_j(t)\, S_j(x) \tag{5.4}$$

where the time dependency of the solution is associated with the nodal unknowns and shape functions are taken to be the same the ones used for steady problems, i.e. functions of space only. Typically shape functions are functions of the master element coordinate ξ, instead of the global coordinate x, but this detail is not important in our discussion here.

Substituting this approximate solution into the weak form we get

$$\int_{\Omega^e} \left[w\left(\sum \frac{dT_j}{dt} S_j\right) + wu\left(\sum T_j \frac{dS_j}{dx}\right) + k\frac{dw}{dx}\left(\sum T_j \frac{dS_j}{dx}\right)\right] dx = \int_{\Omega^e} wf\, dx + \text{B.T.} \tag{5.5}$$

Using GFEM we select a weight function of $w = S_i(x)$ to get the following i^{th} equation of the elemental system

$$\int_{\Omega^e} \left[S_i\left(\sum \frac{dT_j}{dt} S_j\right) + S_i\, u\left(\sum T_j \frac{dS_j}{dx}\right) + k\frac{dS_i}{dx}\left(\sum T_j \frac{dS_j}{dx}\right)\right] dx = \int_{\Omega^e} S_i f\, dx + \text{B.T.} \tag{5.6}$$

Taking the summation sign outside the integral

$$\sum_{j=1}^{NEN} \left[\underbrace{\int_{\Omega^e} S_i S_j\, dx}_{M^e} \right] \frac{dT_j}{dt} + \sum_{j=1}^{NEN} \left[\underbrace{\int_{\Omega^e} \left(S_i\, u\, \frac{dS_j}{dx} + k\, \frac{dS_i}{dx}\, \frac{dS_j}{dx}\right) dx}_{K^e} \right] T_j = \underbrace{\int_{\Omega^e} S_i f\, dx}_{F^e} + \underbrace{B.T.}_{B^e} \tag{5.7}$$

The only difference between this equation and the one obtained for the previously studied steady AD equation is the first term that involves the time derivatives of the nodal unknowns. This final equation can be written in the following compact form

$$[M^e]\{\dot{T}^e\} + [K^e]\{T^e\} = \{F^e\} \tag{5.8}$$

where $\{T^e\}$ is the vector of elemental nodal unknowns and $\{\dot{T}^e\}$ denotes the time derivatives of the nodal unknowns. $[M^e]$, $[K^e]$ and $\{F^e\}$ are the elemental mass matrix, elemental stiffness matrix and elemental force vector. For simplicity elemental boundary integral vector $\{B^e\}$ is included in $\{F^e\}$. When the elemental systems are assembled we obtain the following global system

$$[M]\{\dot{T}\} + [K]\{T\} = \{F\} \tag{5.9}$$

To summarize, for a time dependent problem an extra mass matrix needs to be evaluated. Calculation of other matrices and vectors are the same as steady problems.

5.2 Semi-Discrete Formulation – Time Discretization

Equation (5.9) includes nodal unknowns and their time derivatives. Therefore it is not a set of algebraic equations, but instead a set of ODEs. We still need to discretize the time derivatives of the nodal unknowns. To do this we'll introduce the following discrete time domain where subscript "*s*" denotes time levels.

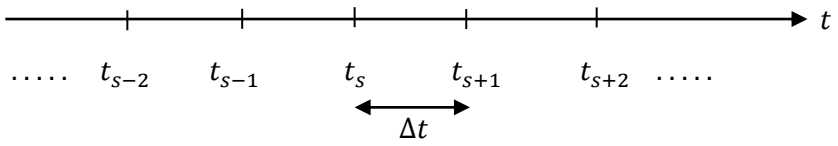


Figure 5.1 Discretization of the time domain

Solution at time level $s = 0$ is given as the initial condition and we'll obtain the solution at other time levels one by one. During any stage of the solution, t_s denotes the current time level where the solution is known and t_{s+1} is the next time level where the solution will be determined. Δt is the time step between time levels s and $s + 1$. For simplicity we will consider Δt to be constant for the whole solution, although it may be more efficient computationally to vary it in time.

5.2.1. Forward Difference (Euler) Scheme

An advantage of semi-discrete formulation is that any of the well known finite difference based time integration schemes can be used to discretize $\{\dot{T}\}$. One of the simplest approximation one can use to discretize $\{\dot{T}\}$ is the following forward difference (Euler) scheme

$$\{\dot{T}\}_s = \frac{\{T\}_{s+1} - \{T\}_s}{\Delta t} + \mathcal{O}(\Delta t) \tag{5.10}$$

where $\{T\}_s$ are the known nodal values of time level s and $\{T\}_{s+1}$ is the unknown vector of the new time level that needs to be calculated. $\mathcal{O}(\Delta t)$ denotes the truncation error, i.e. the accuracy of the scheme, which is first order in this case. In other words truncation error of time discretization decreases linearly with the time step. Substituting this approximation into equation (5.9) written for time step s, we get

$$[M]_s \frac{\{T\}_{s+1} - \{T\}_s}{\Delta t} + [K]_s\{T\}_s = \{F\}_s \tag{5.11}$$

For the AD equation that we are studying and for fluid flow problems that we'll study later, mass matrix is independent of time so we can drop the subscript s from it. But in general stiffness matrix, force vector and boundary condition vector can be functions of time, so let's keep their subscripts. Equation (5.11) can be rearranged as follows to solve for the unknowns at time level $s + 1$

$$\{T\}_{s+1} = [M]^{-1}\left[[M]\{T\}_s + \Delta t\left(\{F\}_s - [K]_s\{T\}_s\right)\right] \tag{5.12}$$

Starting from the known $\{T\}_0$ values, we can use this equation in a time loop to calculate the nodal unknowns at different time levels.

5.2.2. Backward Difference Scheme

Another common way of discretizing the time derivative is to use backward difference scheme given below

$$\{\dot{T}\}_{s+1} = \frac{\{T\}_{s+1} - \{T\}_s}{\Delta t} + \mathcal{O}(\Delta t) \tag{5.13}$$

Substituting this approximation into equation (5.9) written for time step $s+1$, we get (again we'll assume that the mass matrix is independent of time)

$$[M]\frac{\{T\}_{s+1} - \{T\}_s}{\Delta t} + [K]_{s+1}\{T\}_{s+1} = \{F\}_{s+1} \tag{5.14}$$

The unknown vector $\{T\}_{s+1}$ can be solved as follows

$$\{T\}_{s+1} = ([M] + \Delta t[K]_{s+1})^{-1}\,[[M]\,\{T\}_s + \Delta t\,\{F\}_{s+1}\,] \tag{5.15}$$

5.2.3. Crank-Nicolson Scheme

A third commonly used time discretization is known as the Crank-Nicolson scheme, which is based on the following formulation

$$\frac{1}{2}\{\dot{T}\}_s + \frac{1}{2}\{\dot{T}\}_{s+1} = \frac{\{T\}_{s+1} - \{T\}_s}{\Delta t} + \mathcal{O}(\Delta t)^2 \tag{5.16}$$

Which is second order accurate. Crank-Nicolson is kind of an averaging of forward and backward differencing schemes. To use it, let's write equation (5.9) for both time level s and $s+1$ as follows

$$[M]\{\dot{T}\}_s + [K]_s\{T\}_s = \{F\}_s \tag{5.17}$$

$$[M]\{\dot{T}\}_{s+1} + [K]_{s+1}\{T\}_{s+1} = \{F\}_{s+1} \tag{5.18}$$

Multiply these equations by 1/2 , add them up and use equation (5.16) to discretize time derivative terms. Resulting equation can be rearranged to obtain the unknown vector at the new time level as follows

$$\{T\}_{s+1} = \left([M] + \frac{\Delta t}{2}[K]_{s+1}\right)^{-1}\left[\left([M] - \frac{\Delta t}{2}[K]_s\right)\{T\}_s + \frac{\Delta t}{2}(\{F\}_s + \{F\}_{s+1})\right] \tag{5.19}$$

5.2.4. α- Family Schemes

Forward differencing, backward differencing and Crank-Nicolson schemes described above can be generalized as α-family schemes using the following discretization.

$$(\alpha - 1)\{\dot{T}\}_s + \alpha\{\dot{T}\}_{s+1} = \frac{\{T\}_{s+1} - \{T\}_s}{\Delta t}\ , \quad \text{for}\ \ 0 \le \alpha \le 1 \tag{5.20}$$

Similar to what we did for the Crank-Nicolson scheme, we can use Equation (5.20) in equations (5.17) and (5.18) to obtain the following equation that can be used to solve for new unknowns

$$\{T\}_{s+1} = \left[\widehat{K}\right]^{-1}([\overline{K}]\{T\}_s + \{\widehat{F}\}) \tag{5.21}$$

where

$$\left[\widehat{K}\right] = [M] + \alpha\Delta t[K]_{s+1}$$

$$[\overline{K}] = [M] - (1-\alpha)\Delta t[K]_s \tag{5.22}$$

$$\left\{\widehat{F}\right\} = \Delta t\,[\alpha\,\{F\}_{s+1} + (1-\alpha)\{F\}_s]$$

Forward differencing, backward differencing and Crank-Nicolson schemes correspond to the following selections of the α parameter

$$\alpha = \begin{cases} 0 & \text{Forward Differencing (Euler)} \\ 0.5 & \text{Crank-Nicolson} \\ 1 & \text{Backward Differencing} \end{cases} \tag{5.23}$$

5.2.5. Comparison of Implicit and Explicit Time Discretization Schemes and Stability

As seen in equation (5.21), in α family schemes $\left[\widehat{K}\right]$ needs to be inverted. For the forward differencing scheme $\left[\widehat{K}\right]$ is equal to the mass matrix, which is generally time independent. Therefore it needs to be inverted only once, but not at every time level of the numerical solution. However, for backward differencing and Crank-Nicolson schemes $\left[\widehat{K}\right]$ also includes $[K]_{s+1}$, which is likely to be time dependent. Therefore it may be necessary to calculate a new $\left[\widehat{K}\right]$ and invert it at each time step, which is a costly process.

Forward differencing scheme is known as an explicit scheme. Backward differencing and Crank-Nicolson are implicit schemes. In general implicit schemes are computationally more demanding as mentioned above. However, they are also known to be more stable compared to explicit schemes. Stability of a time discretization scheme is about the behavior of errors during the time marching process. If the errors remain bounded, i.e. do not continuously grow in time, the scheme is said to be stable. However, if the scheme allows unlimited growth of errors in time the solution may start to oscillate unphysically and may blow up eventually.

Explicit schemes such as forward differencing are known to be conditionally stable, i.e. time step Δt should be selected smaller than a certain critical value to have stable solutions. In practice this restriction can be too severe, ruining the computational efficiency of the explicit schemes. Implicit schemes such as backward differencing and Crank-Nicolson are unconditionally stable. They do not have critical time step restrictions and can work with larger time steps. However, note that time steps should still be seected small enough to capture the unsteady behavior of the solution accurately. Due to this advantage of being able to work with larger time steps, implicit schemes may be preferred over explicit ones, even if they require more computational work at each time step.

5.2.6. Mass Matrix Lumping

As explained above, unsteady problems are solved step-by-step in a time loop. At each time level a linear algebraic system needs to be solved. Altough explicit schemes could do this in a more efficient manner compared to implicit ones, still the solution of a linear algebraic system at each time level is a costly process. To avoid this lumping can be applied to the mass matrix, convertng it into a diagonal matrix. When the mass matrix becomes diagonal, we no longer need to solve a linear equation system at each time level, insteady the unknowns at the new time level can now be calculated independent of each other. Also with mass lumping critical time step values of conditionally stable schemes become larger. Mass lumping increases computational efficiency considerably, but it also introduces additional numerical errors to the solution and it should be used with care.

Row-sum lumping is the easiest way of obtaining lumped mass matrices. Entries of each row of the mass matrix is summed and the sum is assigned to the diagonal entry of that row. Proportional lumping is another alternative way of lumping the mass matrices [1].

5.2.7. Other Time Discretization Schemes

α-family schemes that are studied in this chapter are not the only possible ways of time discretization. Actually first order forward differencing (Euler scheme) belongs to the family of explicit Adam's Bashforth schemes. Backward differencing and Crank-Nicolson schemes belong to the family of implicit Adam's Moulton schemes. It is possible to study Adam's family schemes to see how higher order explicit and implicit time discretizations can be constructed [2]. Runge-Kutta is another well-known family of schemes used for time discretization [2].

5.3 Sample 1D Unsteady Solution

Consider the unsteady heat diffusion in a 1D domain governed by the following DE

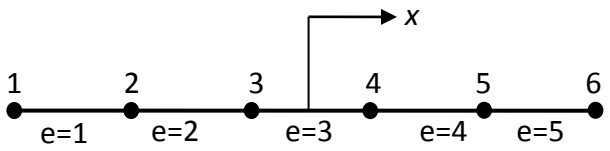
$$\frac{\partial T}{\partial t} - \frac{\partial^2 T}{\partial x^2} = 0\,, \quad -1 \le x \le 1$$

Initial condition : $T(0,x) = (1-x^2)$

Boundary conditions : $T(t,-1) = 0\,, \quad T(t,1) = 0$

The problem can be treated to model the cooling of a 1D bar that is initially heated to have a parabolic temperature distribution with the maximum temperature being at its center. Its ends are kept at a fixed low temperature and the bar loses it to the surrounding through its ends and temperature over it reduces in time until it comes to an equilibrium.

Let's solve this problem using the following mesh of 5 linear elements, each having a length of $h^e = 0.4$



Elemental mass matrix derived in the previous section is

$$M_{ij}^e = \int_{\Omega^e} S_i S_j \, dx = \int_{-1}^{1} S_i S_j \, J^e \, d\xi$$

which will be the same for each element, since all of them are linear elements of the same size. Using the shape functions of 1D linear elements, entries of $[M^e]$ can be evaluated as

$$M_{11}^e = \int_{-1}^{1} \frac{1}{2}(1-\xi) \, \frac{1}{2}(1-\xi) \, \frac{0.4}{2} \, d\xi = \frac{2}{15}$$

$$M_{12}^e = \int_{-1}^{1} \frac{1}{2}(1-\xi) \, \frac{1}{2}(1+\xi) \, \frac{0.4}{2} \, d\xi = \frac{1}{15}$$

$M_{21}^e = M_{12}^e$ (due to symmetry of $[M^e]$)

$$M_{22}^e = \int_{-1}^{1} \frac{1}{2}(1+\xi) \, \frac{1}{2}(1+\xi) \, \frac{0.4}{2} \, d\xi = \frac{2}{15}$$

Therefore elemental mass matrices are

$$[M^e] = \frac{1}{15}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

Assembled global mass matrix is

$$[M] = \frac{1}{15}\begin{bmatrix} 2 & 1 & & & & \\ 1 & 4 & 1 & & & \\ & 1 & 4 & 1 & & \\ & & 1 & 4 & 1 & \\ & & & 1 & 4 & 1 \\ & & & & 1 & 2 \end{bmatrix}$$

Elemental stiffness matrix for the DE of interest is

$$K_{ij}^e = \int_{-1}^{1} \frac{dS_i}{d\xi} \frac{1}{J^e} \, \frac{dS_j}{d\xi} \frac{1}{J^e} \, J^e \, d\xi$$

Considering k to be constant, elemental stiffness matrices will also be the same for all elements. Their entries are

$$K_{11}^e = \int_{-1}^{1} \left(-\frac{1}{2}\right) \frac{1}{0.2} \left(-\frac{1}{2}\right) \frac{1}{0.2} \, 0.2 \, d\xi = 2.5$$

$$K_{12}^e = \int_{-1}^{1} \left(-\frac{1}{2}\right) \frac{1}{0.2} \left(\frac{1}{2}\right) \frac{1}{0.2} \, 0.2 \, d\xi = -2.5$$

$$K_{21}^e = K_{12}^e \quad \text{(due to symmetry of } [K^e]\text{)}$$

$$K_{22}^e = \int_{-1}^{1} \left(\frac{1}{2}\right) \frac{1}{0.2} \left(\frac{1}{2}\right) \frac{1}{0.2} \; 0.2 \, d\xi = 2.5$$

Therefore elemental stiffness matrices are

$$[K^e] = \begin{bmatrix} 2.5 & -2.5 \\ -2.5 & 2.5 \end{bmatrix}$$

and the assembled global stiffness matrix is

$$[K] = \begin{bmatrix} 2.5 & -2.5 & & & & \\ -2.5 & 5 & -2.5 & & & \\ & -2.5 & 5 & -2.5 & & \\ & & -2.5 & 5 & -2.5 & \\ & & & -2.5 & 5 & -2.5 \\ & & & & -2.5 & 2.5 \end{bmatrix}$$

Let's obtain the solution using forward differencing scheme with a time step of $\Delta t = 0.1$. At level $s = 0$ nodal unknown vector $\{T\}_0$ can be obtained from the given initial condition as follows

$$\{T\}_0 = \begin{Bmatrix} 0 \\ 0.64 \\ 0.96 \\ 0.96 \\ 0.64 \\ 0 \end{Bmatrix}$$

To march in time, we need to use the following forward differencing formula derived in the previous section

$$[M]\,\{T\}_{s+1} \;=\; [M]\{T\}_s + \Delta t \,(\,\{F\}_s - [K]_s\{T\}_s\,)$$

For this problem force function on the right hand side of the DE is zero. Also both BCs are of essential type and therefore B_1 and B_6 entries of the elemental boundary integral vector (which is included in $\{F\}_s$) cannot be calculated but they are also not necessary.

To get the solution at the new time level we first need to reduce the above general system to the following 4x4 system by the use of given EBCs

$$\frac{1}{15}\begin{bmatrix} 4 & 1 & & \\ 1 & 4 & 1 & \\ & 1 & 4 & 1 \\ & & 1 & 4 \end{bmatrix}\begin{Bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \end{Bmatrix}_1 = \frac{1}{15}\begin{bmatrix} 4 & 1 & & \\ 1 & 4 & 1 & \\ & 1 & 4 & 1 \\ & & 1 & 4 \end{bmatrix}\begin{Bmatrix} 0.64 \\ 0.96 \\ 0.96 \\ 0.64 \end{Bmatrix} - 0.1\begin{bmatrix} 5 & -2.5 & & \\ -2.5 & 5 & -2.5 & \\ & -2.5 & 5 & -2.5 \\ & & -2.5 & 5 \end{bmatrix}\begin{Bmatrix} 0.64 \\ 0.96 \\ 0.96 \\ 0.64 \end{Bmatrix}$$

Solution at the new time level becomes

$$\begin{Bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \end{Bmatrix}_1 = \begin{Bmatrix} 0.3874 \\ 0.7705 \\ 0.7705 \\ 0.3874 \end{Bmatrix}$$

We can continue like this and calculate one more solution as

$$[M]\,\{T\}_2 = [M]\,\{T\}_1 - 0.1\,[K]\{T\}_1$$

to get

$$\begin{Bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \end{Bmatrix}_2 = \begin{Bmatrix} 0.4588 \\ 0.4689 \\ 0.4689 \\ 0.4588 \end{Bmatrix}$$

Note that forward differencing is a conditionally stable explicit scheme. If we continue a few more time steps we will get unphysical oscillations indicating that we need to lower the time step Δt to obtain a stable solution.

5.4 Exercises

E-5.1. Continue the solution of Section 5.3 and see how the solution blows up. Solve the problem again with the same time step using backward differencing. Does the solution converge to a steady-state?

E-5.2. Modify steady1D.m code so that it can solve time dependent problems with α family schemes. Solve the problem of Section 5.3 with different time steps and determine the critical time step value.

E-5.3. Use the unsteady version of steady1D.m code to solve the problem of Section 5.3 with 50 elements. Is the critical time step value that you calculated in the previous exercise still valid or does the critical time step value depends on the mesh (element length)?

E-5.4. Consider a steel pipeline that is 1 m in diameter and has a wall thickness of 40 mm. The pipe is heavily insulated on the outside, and before the initiation of flow, the walls of the pipe are at a uniform temperature of -20 ℃. With the initiation of flow, hot oil at 60 ℃ is pumped through the pipe, creating a convective condition corresponding to $h = 500\ \mathrm{W/m^2}$ at the inner surface of the pipe. Determine the temperature of the exterior pipe surface covered by the insulation after 8 minutes? Consider the pipe wall to be a plane wall, since its thickness is much less than its diameter. Use multiple meshes and time steps to make sure that your solution is mesh and time step independent. Properties of steel are $\rho = 7832\ \mathrm{kg/m^3}$, $k = 63.9\ \mathrm{W/(mK)}$, $c = 434\ \mathrm{J/(kg\ K)}$.

This problem is taken from reference [3].

E-5.5. A new process for treatment of a special material is to be evaluated. The material is a sphere of radius $r_o = 5\ \mathrm{mm}$, is initially in equilibrium at 400 ℃ in a furnace. It is suddenly removed from the furnace and subjected to a two-step cooling process.

Step 1: Cooling in air at 20 ℃ for a period of time t_a until the center temperature reaches a critical value, $T_a(0, t_a) = 335$ ℃ . For this situation, the convective heat transfer coefficient is $h_a = 10\ \mathrm{W/(m^2K)}$. After the sphere has reached this critical temperature, the second step is initiated.

Step 2: Cooling in a well stirred water bath at 20 °C, with a convective heat transfer coefficient of $h_w = 6000\ \mathrm{W/(m^2K)}$.

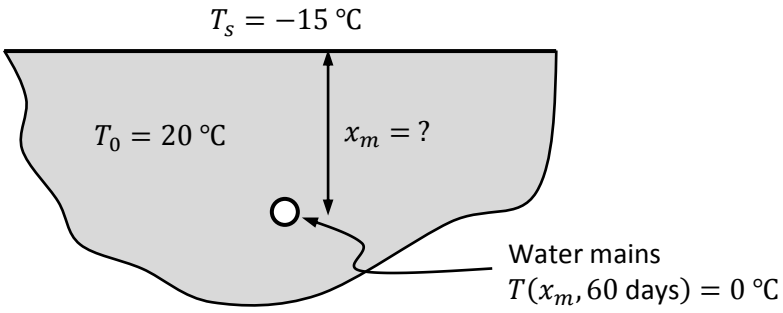
a) Calculate the time t_a required for step 1 of the cooling process to be completed.
b) Calculate the time t_w required during step 2 of the process for the center of the sphere to cool from 335 °C to 50 °C.

Properties of the sphere material are $\rho = 3000\ \mathrm{kg/m^3}$, $k = 20\ \mathrm{W/(mK)}$, $c = 1000\ \mathrm{J/(kg\ K)}$.

This problem is taken from reference [3].

E-5.6. In laying water mains, utilities must be concerned with the possibility of freezing during cold periods. Although the problem of determining the temperature of in soil as a function of time is complicated by changing surface conditions, reasonable estimates can be based on the assumption of constant surface temperature over a prolonged period of cold weather. What minimum burial depth x_m would you recommend to avoid freezing under conditions for which soil, initially at a uniform temperature of 20 °C, is subjected to a constant surface temperature of −15 °C for 60 days? Properties of soil are $\rho = 2050\ \mathrm{kg/m^3}$, $k = 0.52\ \mathrm{W/(mK)}$, $c = 1840\ \mathrm{J/(kg\ K)}$.

This problem is taken from reference [3].



5.5 References

[1] J. N. Reddy, An Introduction to the Finite Element Method, 3rd ed., Mc Graw-Hill, 2005.

[2] S. C. Chapra, R. P. Canale, Numerical Methods for Engineers, 5th ed., Mc Graw-Hill, 2006.

[3] F. P. Incropera, D. P. Dewitt, T. L. Bergman, A. S. Lavine, Fundamentals of Heat and Mass Transfer, 6th ed., John Wiley and Sons, 2007.