The Numerical Method of Lines for Partial Differential Equations

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The method of lines is a general technique for solving partial differential equations (PDEs) by typically using finite difference relationships for the spatial derivatives and ordinary differential equations for the time derivative. William E. Schiesser at Lehigh University has been a major proponent of the numerical method of lines, NMOL.[1] This solution approach can be very useful with undergraduates when this technique is implemented in conjunction with a convenient ODE solver package such as POLYMATH.[2]

A Problem in Unsteady-State Heat Transfer[3]

This approach can be illustrated by considering a problem in unsteady-state heat conduction in a one-dimensional slab with one face insulated and constant thermal conductivity as discussed by Geankoplis.[4]

Unsteady-state heat transfer in a slab in the x direction is described by the partial differential equation

$$\frac{\partial T}{\partial t} = a\,\frac{\partial^2 T}{\partial x^2} \tag{1}$$

where T is the temperature in K, t is the time in s, and α is the thermal diffusivity in m^2/s given by $k/\rho c_p$. In this treatment, the thermal conductivity k in W/m·K, the density ρ in kg/m^3, and the heat capacity c_p in J/kg·K are all considered to be constant.

Consider that a slab of material with a thickness 1.00 m is supported on a nonconducting insulation. This slab is shown in Figure 1. For a numerical problem solution, the slab is divided into N sections with $N + 1$ node points. The slab is initially at a uniform temperature of 100 °C. This gives the initial condition that all the internal node temperatures are known at time $t = 0$.

$$T_n = 100 \text{ for } n = 2 \ldots (N+1) \text{ at } t = 0 \tag{2}$$

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[1] Schiesser, W. E. *The Numerical Method of Lines*, San Diego, CA: Academic Press, 1991.
[2] POLYMATH is a numerical analysis package for IBM-compatible personal computers that is available through the CACHE Corporation. Information can be found at www.polymath-software.com.
[3] This problem is adapted in part from Cutlip, M. B., and M. Shacham *Problem Solving in Chemical Engineering with Numerical Methods*, Upper Saddle River, NJ: Prentice Hall, 1999.
[4] Geankoplis, C. J. *Transport Processes and Unit Operations*, 3rd ed. Englewood Cliffs, NJ: Prentice Hall, 1993.

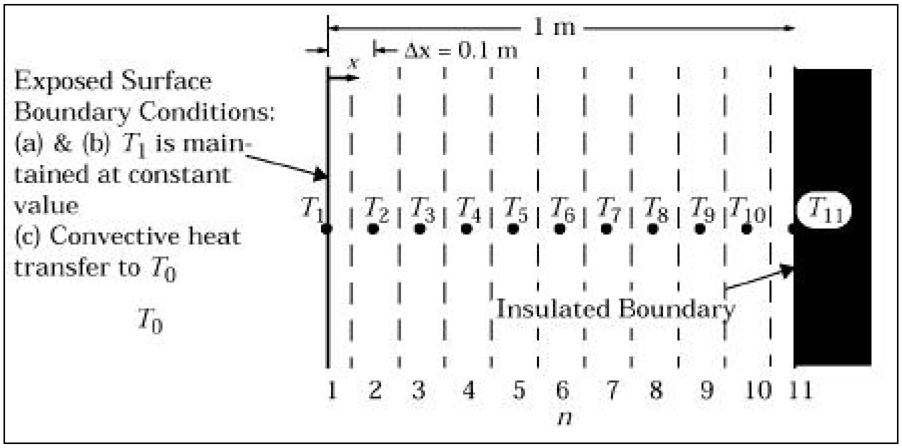

Figure 1 - Unsteady-State Heat Conduction in a One-dimensional Slab

If at time zero the exposed surface is suddenly held constant at a temperature of 0 °C, this gives the boundary condition at node 1:

$$T_1 = 0 \;\text{ for }\; t \geq 0 \tag{3}$$

The other boundary condition is that the insulated boundary at node $N + 1$ allows no heat conduction. Thus

$$\frac{\partial T_{N+1}}{\partial x} = 0 \;\text{ for }\; t \geq 0 \tag{4}$$

Note that this problem is equivalent to having a slab of twice the thickness exposed to the initial temperature on both faces.

Problem (a) - Numerically solve Equation (1) with the initial and boundary conditions of (2), (3), and (4) for the case where $\alpha = 2 \times 10^{-5}$ m²/s and the slab surface is held constant at $T_1 = 0$ °C. This solution should utilize the numerical method of lines with $N = 10$ sections. Plot the temperatures T_2, T_3, T_4, and T_5 as functions of time to 6000 s.

For this problem with $N = 10$ sections of length $\Delta x = 0.1$ m, Equation (1) can be rewritten using a central difference formula for the second derivative as

$$\frac{\partial T_n}{\partial t} = \frac{a}{(\Delta x)^2}\left(T_{n+1} - 2T_n + T_{n-1}\right) \;\text{ for } (2 \leq \text{n} \leq 10) \tag{5}$$

The boundary condition represented by Equation (4) can be written using a second-order backward finite difference as

$$\frac{\partial T_{11}}{\partial t} = \frac{3T_{11} - 4T_{10} + T_9}{2\Delta x} = 0 \tag{6}$$

that can be solved for T_{11} to yield

$$T_{11} = \frac{4T_{10} - T_9}{3} \tag{7}$$

The problem then requires the solution of Equations (3), (5), and (7) which results in nine simultaneous ordinary differential equations and two explicit algebraic equation for the 11 temperatures at the various nodes. This set of equations can be entered into the POLYMATH Simultaneous Differential Equation Solver or some other ODE solver. The resulting equation set for POLYMATH is

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Equations:
d(T2)/d(t)=alpha/deltax^2*(T3-2*T2+T1)
d(T3)/d(t)=alpha/deltax^2*(T4-2*T3+T2)
d(T4)/d(t)=alpha/deltax^2*(T5-2*T4+T3)
d(T5)/d(t)=alpha/deltax^2*(T6-2*T5+T4)
d(T6)/d(t)=alpha/deltax^2*(T7-2*T6+T5)
d(T7)/d(t)=alpha/deltax^2*(T8-2*T7+T6)
d(T8)/d(t)=alpha/deltax^2*(T9-2*T8+T7)
d(T9)/d(t)=alpha/deltax^2*(T10-2*T9+T8)
d(T10)/d(t)=alpha/deltax^2*(T11-2*T10+T9)
alpha=2.e-5
T1=0
T11=(4*T10-T9)/3
deltax=.10
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The initial condition for each of the *T*'s is 100 and the independent variable *t* varies from 0 to 6000. The plots of the temperatures in the first four sections, node points 2 … 5, are shown in Figure 2. The transients in temperatures show an approach to steady state. The numerical results are compared to the hand calculations of a finite difference solution by Geankoplis[4] (pp. 471–3) at the time of 6000 s in Table 1. These results indicate that there is general agreement regarding the problem solution, but differences between the temperatures at corresponding nodes increase as the insulated boundary of the slab is approached.

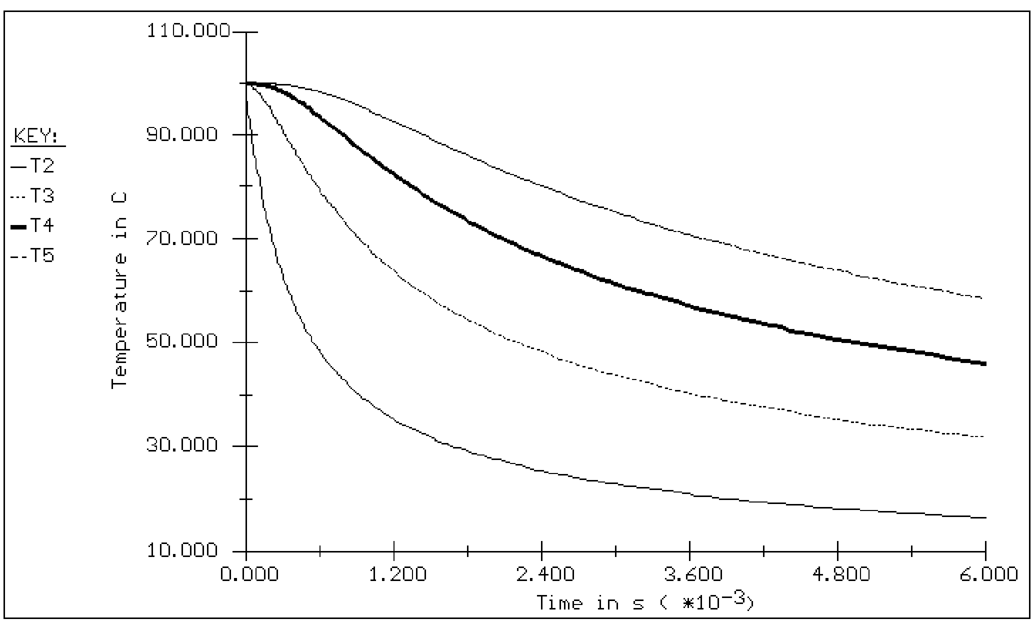

Figure 2 – Temperature Profiles for Unsteady-state Heat Conduction in a One-dimensional Slab

Table 1 – Results for Unsteady-state Heat Transfer in a One-dimensional Slab at t = 6000 s

Distance from Slab Surface in m	Geankoplis[4]		Numerical Method of Lines					
	$Dx = 0.2$m $N = 5$		$\Delta x = 0.1$ m $N = 10$		$\Delta x = 0.05$ m $N = 20$		$\Delta x = 0.0333$ m $N = 30$	
	n	***T***	***n***	***T***	***n***	***T***	***n***	***T***
0	1	0.0	1	0.0	1	0.0	1	0.0
0.2	2	31.25	3	31.71	5	31.68	7	31.67
0.4	3	58.59	5	58.49	9	58.47	13	58.47
0.6	4	78.13	7	77.46	13	77.49	19	77.50
0.8	5	89.84	9	88.22	17	88.29	25	88.31
1.0	6	93.75	11	91.66	21	91.72	31	91.73

Problem (b) - Repeat Problem (a) with 20 sections and compare results with part (a).

The validity of the numerical solution can be investigated by doubling the number of sections for the NMOL solution. This involves adding an additional 10 equations given by the relationship in Equation (5), modifying Equation (7) to calculate T_{21}, and halving Δx. The results for these changes in the POLYMATH equation set are also summarized in Table 1 as are similar results for 30 sections. Here the numerical solutions are similar to the previous solution in part (a) as the temperature profiles are virtually unchanged as the number of section is increased.

Problem (c) - Repeat parts (a) and (b) for the case where heat convection is present at the slab surface. The heat transfer coefficient is h = 25.0 W/m 2 ·K, and the thermal conductivity is k = 10.0 W/m·K.

When convection is considered as the only mode of heat transfer to the surface of the slab, an energy balance can be made at the interface that relates the energy input by convection to the energy output by conduction. Thus at any time for transport normal to the slab surface in the x direction

$$h(T_0 - T_1) = -k \left.\frac{\partial T}{\partial x}\right|_{x=0} \tag{8}$$

where h is the convective heat transfer coefficient in W/m^2·K and T_0 is the ambient temperature.

The preceding energy balance at the slab surface can be used to determine a relationship between the slab surface temperature T_1, the ambient temperature T_0, and the temperatures at internal node points. In this case, the second-order forward difference equation for the first derivative can be applied at the surface

$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = \frac{(-T_3 + 4T_2 - 3T_1)}{2\Delta x} \tag{9}$$

and can be substituted into Equation (8) to yield

$$h(T_0 - T_1) = -k\frac{(-T_3 + 4T_2 - 3T_1)}{2\Delta x} \tag{10}$$

The preceding equation can be solved for T_1 to give

$$T_1 = \frac{2hT_0\Delta x - kT_3 + 4kT_2}{3k + 2h\Delta x} \tag{11}$$

and the above equation can be used to calculate T_1 during the NMOL solution.

The resulting equation set for POLYMATH for Δx = 0.10 m for N = 10 is

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Equations:
d(T2)/d(t)=alpha/deltax^2*(T3-2*T2+T1)
d(T3)/d(t)=alpha/deltax^2*(T4-2*T3+T2)
d(T4)/d(t)=alpha/deltax^2*(T5-2*T4+T3)
d(T5)/d(t)=alpha/deltax^2*(T6-2*T5+T4)
d(T6)/d(t)=alpha/deltax^2*(T7-2*T6+T5)
d(T7)/d(t)=alpha/deltax^2*(T8-2*T7+T6)
d(T8)/d(t)=alpha/deltax^2*(T9-2*T8+T7)
d(T9)/d(t)=alpha/deltax^2*(T10-2*T9+T8)
d(T10)/d(t)=alpha/deltax^2*(T11-2*T10+T9)
alpha=2.e-5
deltax=.10
T11=(4*T10-T9)/3
h=25.
T0=0
k=10.
T1=(2*h*T0*deltax-k*T3+4*k*T2)/(3*k+2*h*deltax)
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The preceding equation set can be integrated to any time t with POLYMATH or another ODE solver. The results at t = 1500 s are summarized in Table 2.

Table 2 – Results for Unsteady-state Heat Transfer with Convection in a One-dimensional Slab at t = 1500 s

Distance from Slab Surface in m	Geankoplis[4]		Numerical Method of Lines					
	Δx = 0.2m N = 5		Δx = 0.1 m N = 10		Δx = 0.05 m N = 20		Δx = 0.0333 m N = 30	
	n	***T***	***n***	***T***	***n***	***T***	***n***	***T***
0	1	64.07	1	64.40	1	64.99	1	65.10
0.2	2	89.07	3	88.13	5	88.77	7	88.90
0.4	3	98.44	5	97.38	9	97.73	13	97.80
0.6	4	100.00	7	99.61	13	99.72	19	99.74
0.8	5	100.00	9	99.96	17	99.98	25	99.98
1.0	6	100.00	11	100.00	21	100.00	31	100.00

There is reasonable agreement between the various NMOL results as the number of sections (smaller Δx) is increased. The slower response of the temperatures within the slab due to the additional convective resistance to heat transfer is evident when the temperatures are compared to those presented in Table 1. Selected temperatures are presented in Figure 3 for the same locations and at the same scale as Figure 2. The delays in the responses of the various temperatures are quite evident.

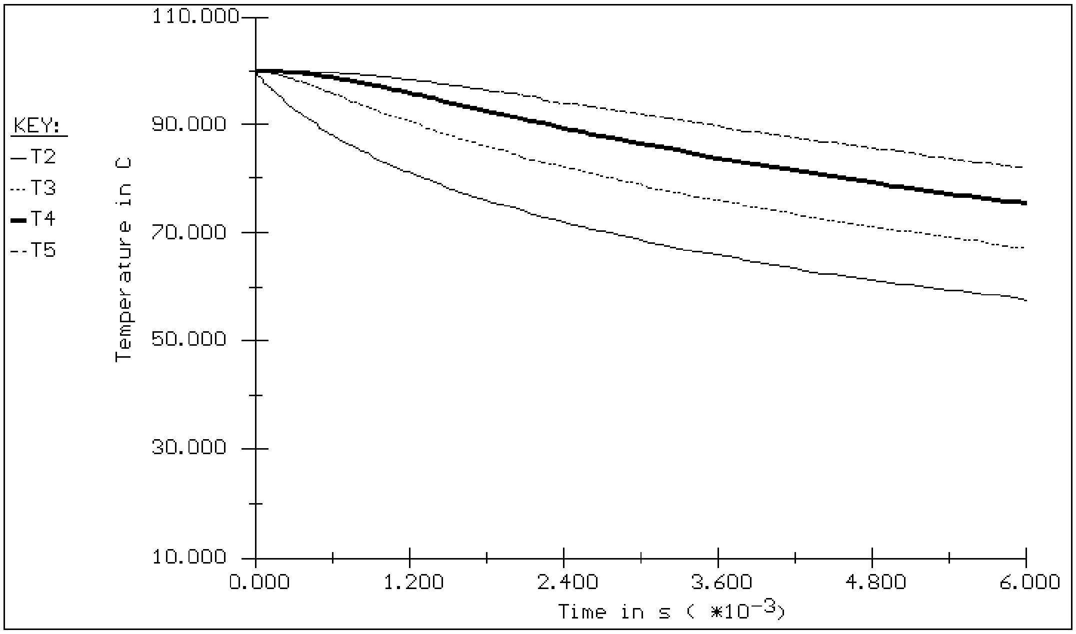

Figure 3 – Temperature Profiles for Unsteady-state Heat Transfer with Convection in a One-dimensional Slab

Problem Extensions

There are a number of extensions to this problem that can be solved with the Numerical Method of Lines. The thermal conductivity of the solid could vary with the local temperature. There could be an initial temperature profile in the solid. Radiative heat transfer to the surface could be considered in addition to the convection. The convective heat transfer coefficient could be a function of the ΔT between the bulk gas and the slab surface. All these possibilities and more can be solved with the NMOL and an ODE solver such as POLYMATH. This type of problem can be used to effectively introduce undergraduate students to transient heat transfer and instruct them to the numerical solution of partial differential equations – a subject area that is not normally considered in a typical curriculum.