Convection and Diffusion

So far, we have neglected the effects of convection in formulating finite volume equation of generalized transport equation. The convection term is represented by $\nabla \cdot (\rho \vec{v} \phi)$ that represents transfer of ($\phi$) due to flow velocity $\vec{V}$. In this chapter, we will discuss the effects of $\vec{V}$ on the transport of property ($\phi$). Although convection term is the only new additional term introduced in addition to other terms we have already discussed in the formulation of diffusion process, inclusion of flow motion creates a substantial difficulty. In most transport processes, convection and diffusion coexist and therefore it is convenient to handle these terms as one unit.

1-D steady convection-diffusion

Consider 1-d, steady-state flow through constant cross-sectional area pipe. Without source, generalized transport equation reduces to

$$\frac{d}{dx} (\rho u \phi) = \frac{d}{dx} (\Gamma \frac{d\phi}{dx})$$

With $\phi = 1.0$ and $\Gamma = 0$, Eq.(1) represents 1-D steady mass conservation equation:

$$\frac{d}{dx} (\rho u) = 0 \quad ; \quad \rho u = \text{constant}$$

Thus 1-D, steady convection-diffusion equation becomes

$$\rho u \frac{d\phi}{dx} = \frac{d}{dx} (\Gamma \frac{d\phi}{dx})$$

For the simplicity of derivation, $\Gamma$ is assumed to be constant. Variable diffusion coefficient can be handled by a similar method [1]. Thus

$$\rho u \frac{d\phi}{dx} = \Gamma \frac{d^2\phi}{dx^2}$$

1
Exact solution of Eq.(4) subject to boundary conditions

\[ \phi(x = 0) = \phi_0 \quad \text{and} \quad \phi(x = L) = \phi_L \]  

is

\[ \frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{\exp\left(\frac{x}{L}\right) - 1}{\exp(P) - 1} \]  

where \( P \) is the generalized Peclet number defined by

\[ P = \frac{\rho u L}{\Gamma} \]  

The nature of the exact solution can be more clearly understood by plotting the variation of \( \phi \) between \( x=0 \) and \( x=L \) as shown in Fig. 1.

\[ \text{Figure 1 Influence of Peclet number (P) on } \phi \]

When \( P=0 \), Eq.(6) reduces to pure diffusion transport case:
Thus $\phi$ varies linearly between $x=0$ and $x=L$ as expected. When Peclet number is positive (i.e., the flow direction is from the left to the right.) the values of $\phi$ along $x$ seem to be influenced by $\phi_0$ that is the upstream value. For extremely large $P$ values, $\phi_0$ prevails almost everywhere except the small region near the right end at $x=L$. This picture is reversed for the negative Peclet number cases. It is apparent that $\phi$ value in the middle point ($x=L/2$) is rarely equal to $(\phi_0 + \phi_L)/2$ and that $\partial\phi/\partial x$ is almost negligible unless Peclet number is small.

**Exponential Scheme**

Eq.(1) can be written as

$$\frac{d}{dx}(J_x) = 0$$

(9)

where $J_x$ is the x-direction flux defined by

$$J_x = \rho u \phi - \Gamma \frac{d\phi}{dx}$$

(10)

that represents both diffusion and convection fluxes. Integrating Eq.(9) over a control volume as was done before, we obtain

$$J_c - J_w = 0$$

(11)

where

$$J_c = (J_x)_c (1x1) = (\rho u \phi)_c - \Gamma_c (\frac{d\phi}{dx})_c (1x1)$$

(12)

and

$$J_w = (J_x)_w (1x1) = (\rho u \phi)_w - \Gamma_w (\frac{d\phi}{dx})_w (1x1)$$

(13)
To evaluate interfacial fluxes at the interface "e" and "w", we use the exact solution given by Eq.(6). For the given geometry and boundary values, the exact solution between the control volumes P and E takes the following form

\[
\frac{\phi - \phi_p}{\phi_e - \phi_p} = \frac{\exp\left(\frac{x}{(\delta x)_e}P\right) - 1}{\exp(P) - 1}
\]

(14)

where x is measured from point "P" as shown in Fig.2.

Thus at the interface "e" we have

\[
\phi_e = \phi_p + (\phi_e - \phi_p) \frac{\exp\left(\frac{x_e}{(\delta x)_e}P_e\right) - 1}{\exp(P_e) - 1}
\]

(15)

Differentiating Eq.(14) with respect to x and evaluating at "e", we get

\[
\left(\frac{d\phi}{dx}\right)_e = (\phi_e - \phi_p) \frac{P_e \exp\left(\frac{x_e}{(\delta x)_e}P_e\right)}{\exp(P_e) - 1}
\]

(16)

where \(P_e\) is the Peclet number at "e" given by
where $F_e$ is the strength of convection and $D_e$ is the diffusion conductance at the interface "e", respectively.

Substituting Eqs.(15) and (16) into Eq.(12), we obtain, after simplification, $J_e$:

$$J_e = F_e \left[ \phi_p + \frac{\phi_p - \phi_E}{\exp(P_e) - 1} \right]$$

(18)

Likewise, at the interface "w", we have

$$J_w = F_w \left[ \phi_w + \frac{\phi_w - \phi_E}{\exp(P_w) - 1} \right]$$

(19)

In Eq.(19), $P_w$ is the local Peclet number at the west interface defined by

$$P_w = \frac{F_w D_e}{(\delta x)_w (1 \times 1)}$$

(20)

where $F_w$ and $D_w$ represent convection strength and diffusion strength at the west interface.

Substituting Eqs.(18),(19) into Eq.(11) and rearranging, we have (left as an exercise),

$$a_P \phi_p = a_E \phi_E + a_w \phi_w$$

(21)

where

$$a_E = \frac{F_e}{\exp(P_e) - 1} = D_e \frac{P_e}{\exp(P_e) - 1}$$

(22a)
In Eq.(22c), $F_e - F_w = 0$ because of mass conservation.

For 1-D, steady convection-diffusion process without source terms, finite volume formulation given by Eq.(21) provides exact solution. All coefficients remain always positive for both positive and negative Peclet numbers. When Peclet number equals to zero, we have

$$a_p = a_E + a_w + (F_e - F_w)$$

(22c)

Generalization of Coefficients

From Eqs.(22a,b), we have

$$a_w = \frac{F_w \exp(P_w)}{\exp(P_w) - 1} = D_w \frac{P_w \exp(P_w)}{\exp(P_w) - 1}$$

(22b)

and

$$a_p = a_E + a_w + (F_e - F_w)$$

(22c)

Behaviors of function $A(P)$ and $B(P)$ are shown in Fig.3. It is easily shown that

$$A(-P) = B(P) \quad \text{and} \quad B(P) = A(P) + P$$

(25a,b)
From these properties, it is possible to represent $A(P)$ and $B(P)$ by

$$A(P) = A(|P|) + \|P,0\|$$  \hspace{1cm} (26a)

and

$$B(P) = A(|P|) + \|P,0\|$$  \hspace{1cm} (26b)

where $\|x,y\|$ means a maximum of $(x,y)$.

Substitution of Eqs.(26a,b) into Eqs.(24a,b), we get

$$a_E = D_e A(|P_e|) + \|F_e,0\|$$  \hspace{1cm} (27a)

and

$$a_w = D_w A(|P_w|) + \|F_w,0\|$$  \hspace{1cm} (27b)
where

$$A(|P|) = \frac{|P|}{\exp(|P|) - 1}$$ \hspace{1cm} (28)

Exponential function in Eq.(28) is approximated by a power-law scheme [Patankar, 1980] to reduce computing time,

$$A(|P|) = \| 0, (1 - 0.1|P|)^5 \|$$ \hspace{1cm} (29)

Fig. 4 shows $A(|P|)$ variations given by Eqs.(28,29) showing good agreement for all Peclet numbers.

In Fig. 4, three additional functional forms of $A(|P|)$ are presented. They are

(a) Central difference scheme:

$$A(|P|) = 1 - \frac{1}{2}|P|$$ \hspace{1cm} (30)

(b) Upwind difference scheme:

$$A(|P|) = 1.0$$ \hspace{1cm} (31)

and

(c) Hybrid scheme:

$$A(|P|) = \| 0, 1 - 0.5 |P| \|$$ \hspace{1cm} (32)

Central difference scheme gives negative $A(|P|)$ values when local Peclet number is greater than 2.0 and the coefficients becomes negative resulting in unrealistic numerical solutions. For the most practical convections, local Peclet number is much greater than 2.0 unless extremely small control volumes are used. Therefore, central difference scheme requires unrealistically large computer time for practical convection problems. Upwind scheme is stable
for all Peclet number since $A(|P|)$ remains positive. However, upwind scheme over-estimates diffusion effects when the Peclet number is large creating numerical diffusion. Hybrid scheme is better than the central and upwind schemes but less accurate than the exponential and power-law schemes.

![Figure 4](image)

Figure 4 Various representation of convection-diffusion coefficient, $A(|P|)$

Quasi 1-dimensional steady convection-diffusion without source is governed by

$$
\frac{1}{A} \frac{d}{dx} (\rho u A \phi) = \frac{1}{A} \frac{d}{dx} (A \Gamma \frac{d\phi}{dx})
$$

(33)

where $A$ is the cross-sectional area perpendicular to the flow direction. If $A$ remains constant Eq.(33) reduces to Eq.(1). Following the procedures as described and utilizing the concept of generalized coefficient, finite volume representation of Eq.(33) can be expressed as

$$
ad_p \phi_p = \alpha_E \phi_E + \alpha_w \phi_W
$$

(34)

where

$$
\alpha_E = D_e A(|p_e|) + \parallel - F_e, 0 \parallel
$$

(35a)
and Cross-sectional area $A_e$ and $A_w$ appear in place of unit area that is assumed for 1-dimensional constant area case. The only difference between the convection-diffusion formulation and pure diffusion formulation is in the coefficients $a_E$, $a_W$ and $a_P$. When the flow speed approaches zero, these coefficients become identical.

As an example of convection-diffusion problem, let us consider a 1-D, steady convection heat transfer. If specific heat $C_P$ is constant, energy equation can be expressed in terms of temperature as

$$\frac{1}{A} \frac{d}{dx} [A(\rho u T - \frac{k}{C_P} \frac{dT}{dx})] = 0$$  \hspace{1cm} (36)$$

If $C_P$ does change, it is more convenient to express energy equation in terms of enthalpy. This subject is discussed later in connection with conjugate heat transfer. Comparison of Eqs.(36) and (33) shows that
By modifying 1-D steady conduction program (std1da.m), we may obtain a 1-D, steady convection-diffusion program. This program is named std1dconv.m.

Example 1

Problem Statement:
Fluid flows steadily from the left tank to the right tank with constant velocity through a constant area pipe. Pipe is insulated. Temperature of fluid along the pipe will depend on the flow speed and the conductivity of fluid. Thermodynamic properties are $C_p=1000$ J/kg.K, $k=0.0407$ W/m.K, $\rho =0.6964$ kg/m$^3$. Flow velocity used is the average velocities; $u= 3$ cm/sec.

Results:
Ten uniform control volumes are used. Local Peclet number is uniform for the present example and is calculated by Eq.(35). For example, when $u=3.0$ cm/s, local Peclet number is

$$ P = \frac{F}{D} = \frac{\rho u \delta x}{k} = \frac{\rho u \delta x}{C_p} = \frac{0.6964 (0.03) (0.01)}{0.0407 / 1000} = 5.13 $$

Three different schemes, central difference, upwind as well as power-law schemes are used for function A($|P|$). When $P=0$, heat transfer between two tanks is pure conduction and temperature distribution is linear in the absence of energy source. All three schemes produce same temperature distributions for small Peclet numbers. When $P=5.13$, Fig. 5 shows central difference scheme becomes unstable and upwind scheme produces too much diffusion in the region near the right tank. Temperature in the left tank prevails all the way except near the right tank. Energy transfer is predominantly controlled by convection.
Figure 5 Temperature distributions for Example 1 with Pec=5.13

Listing of std1d_conv.m

```matlab
%std1d_conv.m
%steady, 1-dimensional conduction-convection with varying cross section area
%nonuniform conductivity and sources. Finite volume formulation
%using matlab program. (By Dr. S. Han, sep 2008)
%with linearized boundary treatment (modified on May 4, 2012)
clear all
close all
clc
iperiodic=0; %not a periodic boundary in x
n=10; %number of control volumes
maxiter=100; %maximum iteration number
np1=n+1;
np2=n+2;
np3=n+3;
%define calculation domain
tl=0.1; %total length of the bar
%dia=2.5e-2; %diameter of the rod
delx=tl/n;
dx=ones(1,np2);
```
dx=delx*dx;
%
if iperiodic==0;%replace fictitious boundary volume size
    dx(1)=1.0e-10;
    dx(np2)=1.0e-10;
else %grid for periodic boundary condition
    dx(1)=dx(np1);
    dx(np2)=dx(2);
end
%
assign x-coordinate
x(1)=0;
for m=1:np2
    x(m+1)=x(m)+dx(m);
end
%
define cross-sectional area
for i=1:np3
    ac(i)=1; %constant cross section
end
%
test of convection-diffusion formulation
plotte=[];
for itest=1:3
    %prescribe intial temperatures for all control volumes
    for i=1:np2
        te(i)=300;
        tep(i)=te(i);
    end
    %iteration for convergence
    iter=0;
    iflag=1;
    %iteration loop for the convergence
    while iflag==1
        %end is at the end of program ********
        %prescribe thermal conductivity
        for i=1:np2
            tk(i)=0.0407;
            ro(i)=0.6964;
            cp(i)=1000;
        end
        %prescribe velocity
        for i=1:np2
            u(i)=0.03;
        end
        %prescribe boundary temperature
        %initialization
        qx0c(1)=0;
        qx0p(1)=0;
        qx0(1)=0;
        qx1c(1)=0;
        qx1p(1)=0;
        qx1(1)=0;
        %boundary type specification
        %bx0(1)=boundary type at x=0: 1(given temperature), 2(given flux), 3(periodic)
        %bx1(1)=boundary type at x=xmax : 1 (given temp), 2(given flux), 3(periodic)
        bx0(1)=1;%specify temperature at x=0
        te(1)=700;%at the left boundary given temperature
        bx1(1)=1; %given convection heat flux, qx1(1)=qx1c(1)+qx1p(1)*te(np2)
        te(np2)=300;
% evaluate the diffusion conductance and source terms
for i=2:nl
% diffusion conductance
ke=tk(i)*tk(i+1)*(dx(i)+dx(i+1))/
(dx(i)*tk(i+1)+dx(i+1)*tk(i));
dc=2.0*ke/cp(i+1)*ac(i+1)/(dx(i)+dx(i+1)); % diffusion conductance
fe=ro(i)*u(i+1)*ac(i+1); % convection strength
pce=abs(fe)/dc; % Péclet number at east interface
temp=1-0.1*pce;
if temp<=0
   temp=0;
else
   temp=temp^5;
end
if itest==1
   ae=dc*max(temp,0)+max(-fe,0); % power-law scheme
elseif itest==2
   ae=dc*(1-0.5*pce)+max(-fe,0); % central scheme
else
   ae=dc+max(-fe,0); % upwind scheme
end
% kw=tk(i)*tk(i-1)*(dx(i)+dx(i-1))/
(dx(i-1)*tk(i)+dx(i)*tk(i-1));
dw=2.0*kw/cp(i)*ac(i)/(dx(i-1)+dx(i));
fw=ro(i)*u(i)*ac(i); % convection strength
pcw=abs(fw)/dw; % Péclet number at east interface
temp=1-0.1*pcw;
if temp<=0
   temp=0;
else
   temp=temp^5;
end
if itest==1
   aw=dw*max(temp,0)+max(fw,0); % power-law scheme
elseif itest==2
   aw=dw*(1-0.5*pcw)+max(fw,0); % central scheme
else
   aw=dw+max(fw,0); % upwind scheme
end
% source term evaluation
sp=0;
sc=0;
ap=ae+aw-sp*dx(i)*0.5*(ac(i+1)+ac(i));
b=sc*dx(i)*0.5*(ac(i)+ac(i+1));
% setting coefficients for tdma matrix
ta(i)=ap;
tb(i)=ae;
tc(i)=aw;
td(i)=b;
% modify using boundary conditions
if i==2 % x=0
   if bx0(1)==1
      td(i)=td(i)+aw*te(1);
   end
   if bx0(1)==2

\[ t_1 = 1 - 0.5 \cdot dx(2)/tk(2) \cdot qx0p(1); \]
\[ t_4 = 0.5 \cdot dx(2)/tk(2) \cdot qx0c(1); \]
\[ ta(i) = ta(i) - tc(i)/t1; \text{% modified coefficient} \]
\[ td(i) = td(i) + tc(i) \cdot t4/t1; \text{% modified coefficient} \]
\[ end \]

\[ if \ i == np1 \text{% at x=xmax} \]
\[ if \ bx1(1) == 1 \]
\[ td(i) = td(i) + ae*te(np2); \]
\[ end \]
\[ if \ bx1(1) == 2 \]
\[ t1 = 1 + 0.5 \cdot dx(np1)/tk(np1) \cdot qx1p(1); \]
\[ t4 = 0.5 \cdot dx(np1)/tk(np1) \cdot qx1c(1); \]
\[ ta(i) = ta(i) - tb(i)/t1; \text{% modified coefficient} \]
\[ td(i) = td(i) - tb(i) \cdot t4/t1; \text{% modified coefficient} \]
\[ end \]
\[ end \]
\[ end \]
\[ end \]
\[ if \ bx0(1) == 3 \]
\[ % solve the simultaneous equations by using tdma \]
\[ nq = n; \]
\[ np1 = nq + 1; \]
\[ nq1 = nq - 1; \]
\[ % forward substitution \]
\[ beta(2) = tb(2)/ta(2); \]
\[ alpa(2) = td(2)/ta(2); \]
\[ for \ i = 3:nq1 \]
\[ beta(i) = tb(i)/(ta(i) - tc(i) \cdot beta(i-1)); \]
\[ alpa(i) = (td(i) + tc(i) \cdot alpa(i-1))/... \]
\[ (ta(i) - tc(i) \cdot beta(i-1)); \]
\[ end \]
\[ % backward substitution \]
\[ dum(nq1) = alpa(nq1); \]
\[ for \ j = 1:nq1 \]
\[ i = nq1 - j; \]
\[ dum(i) = beta(i) \cdot dum(i+1) + alpa(i); \]
\[ end \]
\[ end \]
\[ % end of TDMA \]
\[ % periodic TDMA \]
\[ if \ bx0(1) == 3 \]
\[ % solve equations by CTDMA \]
\[ nq = n; \]
\[ np1 = nq + 1; \]
\[ np2 = nq + 2; \]
\[ % forward substitution \]
\[ cte(2) = tb(2)/ta(2); \]
\[ ctf(2) = tc(2)/ta(2); \]
\[ ctg(2) = td(2)/ta(2); \]
\[ for \ i = 3:nq \]
\[ t1 = ta(i) - tc(i) \cdot cte(i-1); \]
\[ cte(i) = tb(i)/t1; \]
\[ ctf(i) = tc(i) \cdot ctf(i-1)/t1; \]
\[ ctg(i) = (tc(i) \cdot ctg(i-1) + td(i))/t1; \]
\[ end \]
\[ ctp(2) = ta(np1); \]
ctq(2)=tb(nqp1);
ctr(2)=td(nqp1);
for i=3:nq
    ctp(i)=ctp(i-1)-ctq(i-1)*ctf(i-1);
    ctq(i)=ctq(i-1)*cte(i-1);
    ctr(i)=ctq(i-1)*ctg(i-1)+ctr(i-1);
end
t1=(ctq(nq)+tc(nqp1))*ctg(nq)+ctr(nq);
t2=ctp(nq)-(ctq(nq)+tc(nqp1))*(cte(nq)+ctf(nq));
dum(nqp1)=t1/t2;
%backward substitution
for j=2:nq
    i=nqp1-j+1;
    dum(i)=cte(i)*dum(i+1)+ctf(i)*dum(nqp1)+ctg(i);
end
end %end of CTDMA
%update the temperature
for i=2:npl
    te(i)=dum(i);
end
%calculate the boundary temperature or heat flux
if bx0(1)==1 %given temp
    qx0(1)=-tk(2)*(te(2)-te(1))/(0.5*dx(2));
end
if bx0(1)==2 %given heat flux
    te(1)=te(2)+0.5*dx(2)/tk(2)*qx0(1);
end
if bx0(1)==3 %cyclic
    te(1)=te(npl);
    te(np2)=te(2);
end
% if bx1(1)==1 %given temp
%    qx1(1)=qx1c(1)+qx1p(1)*te(np2); %heat flux
end
if bx1(1)==2 %given flux
    te(np2)=te(np1)-0.5*dx(np1)/tk(np1)*qx1(1);
end
%check the convergence
for i=1:np2
    errote(i)=abs(te(i)-tep(i))/te(i);
end
error=1.0e-6;
if (max(errote)>error)
    iter=iter+1;
    tep=te;
    iflag=1;
else
    iflag=0;
end
if iter>maxiter
    break
end % this end goes with the while iflag==1 at the top********
plotte=[plotte te'];
end %this end goes with itest
for i=1:np2
    xc(i)=0.5*(x(i)+x(i+1));
end

fig fprintf('iteration number is %i \n',iter)
%disp('steady state temperatures are');
fprintf('%9.3f \n',te');
plot the result xc.vs.te
plot(xc,plotte(:,1),'-o',xc,plotte(:,2),'-x',xc,plotte(:,3))
xlabel('axis, m'),ylabel('temperature, K')
legend('power-law', 'central', 'upwind')
grid on
title('steady state temp'),xlabel('x(m)'),ylabel('T(K)')

1-D, Transient Convection-Diffusion

We have considered 1-dimensional steady convection-diffusion without source terms. We will now extend the same concept to 1-dimensional transient convection-diffusion problems. The general 1-d convection-diffusion equation may be expressed:

$$\frac{\partial}{\partial t}(\rho \phi) + \frac{\partial}{\partial x}(J_x) = S$$

(38)

where

$$J_x = \rho \ u \ \phi - \Gamma \frac{\partial \phi}{\partial x}$$

(39)

Special case of Eq.(38) is the mass conservation equation:

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho \ u) = 0$$

(40)

Integrating Eq.(38) over a control volume as shown in Fig. 6, we have

$$\frac{(\rho_p \ \phi_P - \rho_p^0 \ \phi_P^0)}{\Delta t} \Delta x(1 \times 1) + J_c - J_w = (S_c + S_p \ \phi_p)\Delta x(1 \times 1)$$

(41)
where superscript "0" indicates previous time-level properties and \( J_e \) and \( J_w \) are \( x \)-direction convection-diffusion flux times the cross-sectional area at the interfaces "e" and "w" respectively;

\[
J_e = (\rho u \phi - \Gamma \frac{\partial \phi}{\partial x})_{e} (1 \times 1)
\]  

and

\[
J_w = (\rho u \phi - \Gamma \frac{\partial \phi}{\partial x})_{w} (1 \times 1)
\]

Integrating the continuity equation, Eq.(40), over the same control volume, we obtain

\[
\frac{(\rho_p - \rho_p^0)\Delta x (1 \times 1)}{\Delta t} + F_e - F_w = 0
\]  

where \( F_e \), and \( F_w \) are convection strength at the east and west interfaces, respectively.

![Figure 6 Control volume for \( \phi_p \)]

Now, multiply \( \phi_p \) to Eq.(43) and subtract it from Eq.(41). The resulting equation is

\[
(\phi_p - \phi_p^0) \frac{\rho_p^0 \Delta x (1 \times 1)}{\Delta t} + (J_e - F_e \phi_p) - (J_w - F_w \phi_p) = (S_e + S_p \phi_p) \Delta x (1 \times 1)
\]  

(44)
Recall that from Eq. (18), we have
\[
J_c - F_c \phi_p = \frac{F_c}{\exp(P_c) - 1} (\phi_p - \phi_E) = D_c \frac{P_c}{\exp(P_c) - 1} (\phi_p - \phi_E)
\]

Using Eq. (24a), this can be written as
\[
J_c - F_c \phi_p = D_c A(P_c) (\phi_p - \phi_E) = a_E (\phi_p - \phi_E) \quad (45)
\]

Likewise, using Eqs. (19) and (24b), we get
\[
J_w - F_w \phi_p = a_w (\phi_w - \phi_p) \quad (46)
\]

Substituting Eqs. (45) and (46) into Eq. (44), we obtain finite volume formulation of 1-dimensional transient convection-diffusion equation:
\[
a_p \phi_p = a_E \phi_E + a_w \phi_w + b \quad (47)
\]

where
\[
a_E = D_c A(P_c) + \parallel F_c, 0 \parallel \quad (48a)
\]
\[
a_w = D_w A(P_w) + \parallel F_w, 0 \parallel \quad (48b)
\]
\[
a_p = \frac{\rho_p^0 \Delta x (1 \times 1)}{\Delta t} \quad (48c)
\]
\[
b = \Delta x (1 \times 1) \times a_p \phi_p^0 \quad (48d)
\]
and $P_e$ and $P_w$ are Peclet number at the east and west interface, respectively.

Fully-implicit scheme is used in the present formulation as discussed in pure diffusion process. It was observed that time step size should be comparable to CFL stability criterion to obtain time accurate transient solution. Following the same procedure for the convection-diffusion process, the following condition must be met to ensure positive coefficient requirement

$$-a_e - a_w + a_p^0 \geq 0$$

Using Eqs.(24a) and (24b), this can be written, assuming $P_e = P_w = P$ for convenience,

$$-DP \left[ \frac{1 + \exp(P)}{\exp(P) - 1} \right] + \frac{\rho \Delta x}{\Delta t} \geq 0$$

Rearranging this we have

$$\Delta t \leq \frac{\rho \Delta x}{D} \left[ \frac{\exp(P) - 1}{P(\exp(P) + 1)} \right]$$

(49)

When Peclet number approaches to zero Eq.(49) reduces to

$$\Delta t \leq \frac{\rho \Delta x}{2D} = \frac{\rho \Delta x}{2} \frac{\Gamma}{\Delta x}$$
which is identical to pure diffusion case.

If local Peclet number is greater than 2, Eq.(49) can be approximated by

$$\Delta t \leq \frac{\rho \Delta x}{D} \frac{1}{P} \quad \text{for} \quad P \geq 2$$  \hspace{1cm} (50)

Thus the optimum time step for transient convection problem should be in the same order as given by Eq.(50).

A quasi-one-dimensional transient convection-conduction heat transfer in terms of temperature may be expressed by

$$\frac{1}{A} \frac{\partial}{\partial t} (\rho A T) + \frac{1}{A} \frac{\partial}{\partial x} \left[ A(\rho u T - \frac{k}{C_p} \frac{\partial T}{\partial x}) \right] = S$$ \hspace{1cm} (51)

It is assumed that $C_p$ is constant and $A=A(x)$ in general. Comparing Eq.(51) with Eq.(38), we have

$$\phi = T \quad \text{and} \quad \Gamma = \frac{k}{C_p}$$

Also constant cross-sectional area (1x1) is replaced by $A(x)$. Finite volume equation is similar to Eq.(47) except the change in cross-sectional area $A(x)$.

**Boundary Conditions**

Boundary treatment of convection-diffusion problems follows a similar approach as used in pure diffusion cases. We will discuss implementation of boundary conditions in terms of convection-conduction problems. The governing differential equation is given by Eq.(51). Finite volume equation in index notation is
where $T_1$ and $T_{N+2}$ are boundary temperatures and must be provided by boundary conditions. If boundary temperatures are known, imposition of boundary condition is straightforward. Other types of boundary conditions involving convection and diffusion at the boundary can be encountered and we need to develop a general method to handle such boundary conditions as was done for conduction cases.

Consider boundary control volumes near the left boundary as shown in Fig. 7. Taking an energy balance at the fictitious control volume, we have

$$a_2 T_2 = b_2 T_1 + c_2 T_1 + d_2$$

$$a_3 T_3 = b_3 T_1 + c_3 T_2 + d_3$$

.............

$$a_i T_i = b_i T_{i+1} + c_i T_{i+1} + d_i$$

............... (52)

$$a_N T_N = b_N T_{N+1} + c_N T_{N+1} + d_N$$

$$a_{N+1} T_{N+1} = b_{N+1} T_{N+2} + c_{N+1} T_N + d_{N+1}$$

where $T_1$ and $T_{N+2}$ are boundary temperatures and must be provided by boundary conditions. If boundary temperatures are known, imposition of boundary condition is straightforward. Other types of boundary conditions involving convection and diffusion at the boundary can be encountered and we need to develop a general method to handle such boundary conditions as was done for conduction cases.

Consider boundary control volumes near the left boundary as shown in Fig. 7. Taking an energy balance at the fictitious control volume, we have

$$q_B'' = -k_w \left( \frac{\partial T}{\partial x} \right)_w$$

(53)

where $q_B''$ is the convection-diffusion flux entering through the boundary, taken positive along the positive $x$-direction. Appropriate form of $q_B$ depends on the physical problems.

![Figure 7 Energy balance at x=0](image)

Temperature gradient at the west interface, Eq.(53) becomes,
Solving for $T_1$ from Eq.(54), we get

$$T_1 = T_2 + \frac{1}{2} \left[ \frac{\Delta x_2}{k_2} q_{B'} \right]$$  \hspace{1cm} (55)$$

By a similar procedure at the right boundary, we have

$$T_{N+2} = T_{N+1} - \frac{1}{2} \left[ \frac{\Delta x_{N+1}}{k_{N+1}} q_{B'} \right]$$  \hspace{1cm} (56)$$

where $q_{B'}$ is convection-conduction flux at the right boundary and taken positive along the positive $x$-direction. For most of convection dominated problems, $q_B$ can be taken zero implying that $T_{n+2} = T_{n+1}$.

Periodic boundary condition is treated by the same method as discussed in conduction and does not require additional considerations.

**A Closer Look at Diffusivity in Convection-Diffusion**

In Eq.(51), $k/C_p$ is considered a diffusion coefficient in the formulation of convection-conduction formulation. In real physical process, however, $k$ is the diffusion coefficient related to thermal conduction expressed by Fourier's law. Therefore, when we calculate interfacial thermal conductivity, we should consider interfacial conductivity, $k$ and not $k/C_p$. If $C_p$ is constant as in Example 1, there is no difference whether $k$ or $k/C_p$ is used for diffusion process through the interfaces. Consider the energy balance in a control volume as shown in Fig. 8.

$$q_{S'} = -k_2 \left[ \frac{T_2 - T_1}{0.5 \Delta x_2 + \Delta x_1} \right]$$  \hspace{1cm} (54)$$

Figure 8 A control volume in quasi 1-D convection-diffusion
It can be shown that the energy balance equation is (left as an exercise)

\[ \frac{\partial}{\partial t} (\rho c_p T) + \frac{1}{A} \frac{\partial}{\partial x} \left[ A \left( \rho u c_p T - k \frac{\partial T}{\partial x} \right) \right] = \dot{q} + \frac{q_s P}{A} \]  \hspace{1cm} (57)

P is the wetted perimeter of the cross section, u is the velocity, and \( \dot{q} \) is the energy generation rate per unit volume. If \( c_p \) is constant and A is constant (57) reduces to

\[ \frac{\partial}{\partial t} (\rho T) + \frac{1}{A} \frac{\partial}{\partial x} \left[ (\rho u T - \frac{k}{c_p} \frac{\partial T}{\partial x}) \right] = \frac{1}{c_p} \left( \dot{q} + \frac{q_s P}{A} \right) \]  \hspace{1cm} (58)

If \( c_p \) is not constant, energy conservation for convection-conduction process is more conveniently described in terms of enthalpy and Eq. (57) can be written, with A=constant,

\[ \frac{\partial \rho h}{\partial t} + \frac{\partial}{\partial x} \left( \rho u h - \frac{k}{c_p} \frac{\partial h}{\partial x} \right) = S^h \]  \hspace{1cm} (59)

where \( h \) is assumed to be

\[ dh = C_p(T) \, dT \]  \hspace{1cm} (60)

which is valid for ideal gas or incompressible substance with moderate pressure change.

Note that in Eq.(59), \( h \) is the dependent variable, i.e., \( \phi=h \), not \( T \) and \( S^h \) is source terms represented by right side of Eq.(57).

For 1-dimensional steady heat conduction without any source, Eq. (59) reduces to

\[ \frac{d}{dx} \left( \frac{k}{C_p} \frac{dh}{dx} \right) = \frac{d}{dx} \left[ \kappa \frac{dT}{dx} \right] = 0 \]  \hspace{1cm} (61)

Integrating Eq.(61) over a control volume as shown in Fig. 9, we have

\[ \frac{\kappa_e}{(\Delta x)_e} (T_E - T_p) - \frac{\kappa_w}{(\Delta x)_w} (T_p - T_w) = \frac{\kappa_e}{(\Delta x)_e} \left( \frac{h_E}{C_p} - \frac{h_p}{C_p} \right) - \frac{\kappa_w}{(\Delta x)_w} \left( \frac{h_p}{C_p} - \frac{h_w}{C_p} \right) = 0 \]  \hspace{1cm} (62)

In writing Eq.(61) it is assumed that

\[ h = C_p T \]
Figure 9 Control volumes with variable $C_P$

Collecting terms in Eq. (62), we have

$$a_P h_P = a_E h_E + a_W h_W$$

(63)

where

$$a_E = D_e = \frac{k_e}{(\delta x)_e C_{P_e}}$$

$$a_W = D_w = \frac{k_w}{(\delta x)_w C_{P_w}}$$

(64a; b; c)

$$a_P = D_e \left( \frac{C_{P_w}}{C_{P_e}} \right) + D_w \left( \frac{C_{P_w}}{C_{P_P}} \right)$$

Interfacial conductivity at the interfaces is to be evaluated as before.

By extending this concept to convection-diffusion equation, Eq.(59), we may write
where \( D_e \) and \( D_w \) are given by Eqs.(64a;b).

Thus in convection-diffusion formulation, generalized diffusion coefficient \( \Gamma \) is made of a physical diffusion coefficient times other property. For example, in convection-conduction formulation, \( k \) and \( 1/C_p \). This formulation is valid as well if \( T \) is dependent variable when \( c_p \) is constant except the source term is \( S^T = S^h/C_p \) as shown in Eq. (58).

**Transient 1-D, Convection-Diffusion Program**

A transient 1-d convection-diffusion program (conv1d.m) including time dependent term and variable specific heat is created by modifying std1d_conv.m. In this program area change, \( A(x) \), is also included.

Example 2

Problem description:
Consider temperature distribution in the pipe as discussed in Example 1. We want to calculate transient temperature distribution in the pipe when the temperature in the left tank is suddenly raised to 700 K over the initial temperature of 300 K through the system. Density, conductivity and \( c_p \) are all assumed to be constant. The governing convection-diffusion equation for this example is obtained by dividing Eq.(59) by \( c_p \). The resulting equation is

\[
\frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x}\left( \rho u T - \frac{\kappa}{C_p} \frac{\partial T}{\partial x} \right) = S^r = \frac{S^h}{C_p}
\]  

(66)

Diffusion coefficient is the conductivity and other property multiplied to \( k \) to form a
general diffusion coefficient is $1/C_P$.

Ten uniform control volumes are used. Area is assumed to be constant. Velocity is 0.03 m/s. Thus the local Peclet number is 5.13 as in Example 1. Time step satisfying CFL condition estimated by Eq.(49) is 0.33 sec. To catch the transient behavior 0.1 sec is used. Boundary conditions are known boundary temperatures at $x=0$ and $x=L$. There are no source terms, $Sc=Sp=0$. Listing of conv1d_input_sample.m is shown below. The steady state solution is in agreement with the result in Example 1, as expected.

![Transient temperature](image)

**Figure 9 Transient temperature in the pipe flow, Pec=5.13**

**Listing of conv1d_input_example.m**

```matlab
%conv1d_input_example.m
%transient, 1-dimensional convection-diffusion with varying cross section area
%n,nonuniform properties and sources. Finite volume formulation
%using matlab program. (By Dr. S. Han, Sep 25, 2007)
%modified to include all types of boundary conditions. (May 5, 2012)
%modified March 2013.
```
%list of symbols:
%   ac=sectional area
%   dt=time step
%   iflag=0 (solution converged), iflag=1 (solution is not converged)
%   iter=iteration counter
%   maxiter= maximum iteration allowed in a time step
%   n=number of control volumes
%   te=temperature at new time level
%   tep=projected temperature at new time level
%   te0=temperature at old time level
%   tk=diffusion coefficent(thermal conductivity)
%   tstop=time to stop computation
%   x=independent variable (spatial coordinate), dx=delta x
% function figure1.m: plots line graph x vs te

clear all
close all
clc
%specify periodic boundary
iperiodic=0; %not a periodic boundary; 1=periodic boundary
%specify the number of control volumes
n=20; %number of control volumes
maxiter=10; % maximum number iteration allowed in each time step
mwrite=4; %print results at every 10 time steps
dt=0.1; %time step
tstop=10; %time to stop the calculation
np1=n+1;
np2=n+2;
np3=n+3;
re=1.0; %relaxation coefficient for simultaneous equation
%define calculation domain
dx=ones(1,np2);
tl=0.1;
delx=tl/n;
dx=delx*dx;
if iperiodic==0
    dx(1,1)=1.0e-10;
dx(1,np2)=1.0e-10;
else
    dx(1,1)=dx(1,np1);
dx(1,np2)=dx(1,2);
end
%x(1,1)=0;
for i=1:np2
    x(1,i+1)=x(1,i)+dx(1,i);
end
%define cross sectional area
for i=1:np3
    ac(1,i)=1;
end
%prescribe intitial temperatures
for i=1:np2
    te0(i)=300;
\[ te(i) = te0(1,i); \]
\[ tep(i) = te(1,i); \quad \text{%predicted value at the next iteration} \]

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% time loop begins here
\[ t = 0; \quad \text{%starting time} \]
\[ plotte = [te']; \quad \text{%save temperatures for plot} \]
\[ iwrite = 1; \quad \text{%printout counter, iwrite<mwrite then skip printout} \]
while \( t < tstop \)
  % iteration for convergence
  iter = 0;
  iflag = 1;
  %iteration loop for the convergence
  while iflag == 1
    % end is at the end of program ****************(1)
    % prescribe thermal property
    for \( i = 1 : np2 \)
      \[ tk(1,i) = 0.0407; \quad \text{%conductivity} \]
      \[ ro(1,i) = 0.6964; \quad \text{%density} \]
      \[ cp(1,i) = 1000; \quad \text{%specific heat} \]
    end
    % prescribe velocity********************This an addition
    for \( i = 1 : np3 \)
      \[ u(i) = 0.03; \quad \text{%velocity in m/s} \]
    end
    % incorporate boundary conditions calling boundy.
    % initialize fluxes
    \[ qx0c = zeros(1); \]
    \[ qx0p = zeros(1); \]
    \[ qx0 = zeros(1); \]
    \[ qxlc = zeros(1); \]
    \[ qxlp = zeros(1); \]
    \[ qx1c = zeros(1); \]
    \[ qx1p = zeros(1); \]
    \[ qx1 = zeros(1); \]
    % bx0(l)=1,2,3(known temperature, known flux, periodic) at x=0
    % bx1(l)=1,2,3 (same) at x=xmax
    % at x=0
    bx0(1) = 1;
    te(1) = 700; \quad %base temperature
    % at x=xmax
    bx1(1) = 1;
    te(np2) = 300;
    % incorporate source terms .
    for \( i = 1 : np2 \)
      \[ sp(1,i) = 0; \]
      \[ sc(1,i) = 0; \]
    end
    % solve equations calling conv1dInvariant.m
    conv1dInvariant;
    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%end % this end goes with the while iflag==1 at the top***************
  %
  %advance to next time
  \[ t = t + dt; \quad \text{%increase time to next level} \]
  for \( i = 1 : np2 \)
    \[ te0(1,i) = te(1,i); \quad \text{%reinitialize variable} \]
    \[ tep(1,i) = te0(1,i); \]
end
%write the results at this time?
if iwrite>mwrite
fprintf('iteration number is %i \n',iter)
%disp('transient temperatures are')
fprintf('%9.3f\n',te)
plotte=[plotte te];
iwrite=0;
end
end %this end goes with time loop while t<tstop
%plot the result x.vs.te by calling function figure1
figure1(n,x,plotte);

Example 3. Crystal Growth Process

One of the popular methods of growing single large crystal is to use Bridgeman method as depicted in Fig.9.12. Polycrystalline rod is slowly pulled through a region where radiation beam melt the solid momentarily into liquid and resolidifies into crystal material. Polycrystalline material contains impurity called dopant to control electrical properties of the crystal. Mass fraction of dopant is usually very small in the order of few percent. In the melt region, binary mass transfer occurs between the carrier fluid and the dopant material. The governing convection-diffusion equation is [Geankoplis, 1972],

\[
\frac{\partial (\rho W_A)}{\partial t} + \frac{\partial}{\partial x} \left( \rho u W_A - \rho D_{AB} \frac{\partial W_A}{\partial x} \right) = 0 \tag{67}
\]

where \( W_A (\frac{\rho_A}{\rho}) \) is the mass fraction of dopant, \( \rho \) is the density of the mixture that is assumed to be constant and \( D_{AB} \) is the binary mass diffusivity.
Figure 10 Bridgeman method

Boundary conditions can be derived by taking mass balance for the dopant material. At the interface between feed rod/melt (x=0), we have

\[ V_x W_A^0 = V_x W_A - D_{AB} \frac{\partial W_A}{\partial x} \]  

(68)

where \( V_x \) is the pulling speed and \( W_A^0 \) is the known dopant concentration in the feed rod. It is assumed there is no mass diffusion into the solid. At the crystal/melt interface (x=L), mass balance for dopant is

\[ -D_{AB} \frac{\partial W_A}{\partial x} + V_x W_A = V_x W_A' \]  

(69)

where \( W_A' \) is the mass fraction of dopant in the crystal. It is again assumed there is no mass diffusion into the solid. \( W_A' \) depends on the segregation coefficient \( (K_0) \)

\[ K_0 = \frac{W_A'}{W_A} \]  

(70)

which is a property of the mixture.

Eq.(67) shows that

\[ \phi = W_A \quad \text{and} \quad \Gamma = \rho D_{AB} \]  

(71)

Rearranging Eq.(68) we have

\[ V_x W_A^0 - V_x W_A = D_{AB} \frac{\partial W_A}{\partial x} \]  

(72)

The LHS of Eq.(72) can be considered virtual mass flux entering through the left boundary. Thus
Likewise on the right boundary, rearranging Eq.(69), we have

\[ q'' = q_c + q_p W_A \]

\[ q_c = V_x W_A^0 \quad \text{and} \quad q_p = - V_x \]

Thus, at \( x=L \),

\[ q_c = - V_x W_{A,N+1} \quad \text{and} \quad q_p = V_x K_0 \]

(75)

It is useful to compare numerical solution with exact solution. If \( D_{AB} \) is constant, Eq.(9.80) reduces to, for steady-state,

\[ V_x \frac{dW_A}{dx} - D_{AB} \frac{d^2 W_A}{dx^2} = 0 \]

(76)

Introducing

\[ z = \frac{x}{L} \quad \text{and} \quad C = \frac{W_A}{W_A^0} \]

(77)

into Eq.(9.89), we get

\[ \text{Pe} \frac{dC}{dz} - \frac{d^2 C}{dz^2} = 0 \]

(78)

where \( \text{Pe}=V_x L/D_{AB} \) and \( L \) is the melt length. Non-dimensionalized boundary conditions are
\[ \frac{\partial C}{\partial z} = \text{Pe}(C-1) \quad \text{at } z = 0 \] (79)

\[ \frac{\partial C}{\partial z} = \text{Pe}(1 - K_0) C \quad \text{at } z = 1 \]

Exact solution is (left as an exercise)

\[ C(z) = 1 + \frac{1 - K_0}{K_0} \exp[\text{Pe}(z - 1)] \] (80)

Physical description:
Cylindrical shaped polycrystalline material with dopant concentration of 3 % is used to obtain single crystal. Density of the material is 1000 kg/m$^3$, and binary mass diffusivity is $D_{AB} = 16 \times 10^{-7}$ m$^2$/s. Pulling velocity is $1.39 \times 10^{-5}$ m/s (5 cm/hr). Length of the melt region is 3 cm. The segregation coefficient is 0.1. It is assumed that the temperature of polycrystalline rod is slightly below its melting temperature before entering the heating region.

Number of control volumes is 20. Clustering of control volume near the melt/crystal interface can be accomplished by using [Patankar, 1991],

\[ \frac{x(I)}{x_{\text{max}}} = 1 - \left(1 - \frac{I - 2}{\text{NP}2 - 2}\right)^n \]

where $n > 1.0$ gives clustering near $x_{\text{max}}$. Presently $n=1.3$ is used. To have time accurate solution, time step must satisfy Eq.(49). Local Peclet number is about 0.5 and the time step is controlled by local diffusion and is about 5.4 sec. However, this time step requires excessive number of iterations since the process takes a very long time to reach a steady state. A time step 60 sec is taken which is much larger than CFL condition.

Initial concentration is 0.03. Pulling velocity is 5 cm/hr. Boundary conditions are given fluxes. There is no source.

Results:
Steady state is reached at about 141000 sec (4 hrs). Up to this time therefore dopant concentration in the crystal will be less than 3 %. Accuracy of transient solution is however is questionable because of large time step used. Comparison of steady state solution with exact solution is very good.
Comments:

In actual crystal growth, heat transfer from the external source is important and the flow, temperature and concentration fields are at least two dimensional axisymmetric.

%conv1d_input_crystal.m
%transient, 1-dimensional convection-diffusion with varying cross section area
%nonuniform properties and sources. Finite volume formulation
%using matlab program. (By Dr. S. Han, Sep 25, 2007)
%modified to include all types of boundary conditions. (May 5, 2012)
%modified on March 2013
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%list of symbols:
% ac=cross-sectional area
% dt=time step
% iflag=0 (solution converged) ,iflag=1 (solution is not converged)
% iter=iteration counter
% maxiter= maximum iteration allowed in a time step
% n=number of control volumes
% te=temperature at new time level
% tep=projected temperature at new time level
% te0=temperature at old time level
% tk=diffusion coefficent(thermal conductivity)
% tstop=time to stop computation
% x=independent variable (spatial coordinate), dx=delta x
% function figure1.m: plots line graph x vs te
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%te=WA, mass fraction of dopanrt material
clear all
close all
clear
%specify periodic boundary
iperiodic=0; %not a periodic boundary; 1=periodic boundary
%specify the number of control volumes
n=20; %number of control volumes
maxiter=10; %maximum iteration allowed in each time step
mwrite=100; %print results at every 10 time steps
dt=60; %time step
tstop=180000; %time to stop the calculation
np1=n+1;
np2=n+2;
np3=n+3;
re=1.0; %relaxation coefficient for simultaneous equation
%define calculation domain
dx=ones(1,np2);
tl=0.03; %total length of the melt
%grid clustering is used
small=1.0e-10;
pwrn=1.3;
for i=2:np2
    temp=1-(i-2)/(np2-2);
    x(1,i)=tl*(1-temp^pwrn)+small;
end
x(1,1)=x(1,2)-small;
x(1,np3)=x(1,np2)+small;
for i=1:np2
    dx(1,i)=x(1,i+1)-x(1,i);
end
if iperiodic==1
    dx(1,1)=dx(1,np1);
    dx(1,np2)=dx(1,2);
end
%define cross sectional area
for i=1:np3
    ac(1,i)=1;
end
%%%%%%%%%%%%%%%%%%%%%%%%%
%prescribe intitial values
for i=1:np2
    te0(i)=0.03;
    te(i)=te0(1,i);
    tep(i)=te(1,i); %predicted value at the next iteration
end
%%%%%%%%%%%%%%%%%%%%%%%%%
%time loop begins here
plotte=[te'];%save temperatures for plot
iwrite=1; %printout counter, iwrite<mwrite then skip printout
while t<tstop
    %iteration for convergence
    iter=0;
    iflag=1;
    %iteration loop for the convergence
    while iflag==1
        % end is at the end of program ********************
        %prescribe property
        for i=1:np2
            tk(1,i)=4.16e-7;%binary diffusivity, D_AB
            ro(1,i)=1000;%density
            cp(1,i)=1/ro(1,i);%ro*D_AB
        end
        %prescribe velocity
        for i=1:np3
            u(i)=1.39e-5; % pulling velocity in m/s
        end
        %incorporate boundary conditions .
        %initialize fluxes
        qx0c=zeros(1);
        qx0p=zeros(1);
        qx0=zeros(1);
        qx1c=zeros(1);
        qx1p=zeros(1);
        qx1=zeros(1);
        %bx0(1)=1,2,3(known temperature, known flux, periodic) at x=0
        %bx1(1)=1,2,3 (same) at x=xmax
        vx=1.39e-5;%pulling speed
        wa0=0.03;%concentration in polycrystal
        k0=0.1;%segregation coefficient
        %at x=0
bx0(1)=2;
qx0c(1)=vx*wa0;
qx0p(1)=-vx;
qx0(1)=qx0c(1)+qx0p(1)*te(1);
%at x=xmax
bx1(1)=2;
qx1c(1)=-vx*te(np1);
qx1p(1)=vx*k0;
qx1(1)=qx1p(1)*te(np2);
%incorporate source terms
for i=1:np2
    sp(1,i)=0;
    sc(1,i)=0;
end
%solve equations.
conv1d_invariant;

end %this end goes with the while iflag==1 at the top******************
%
%advance to next time
t=t+dt;%increase time to next level
for i=1:np2
    te0(1,i)=te(1,i);%reinitialize variable
tep(1,i)=te0(1,i);
end
%write the results at this time?
if iwrite>mwrite
%print the results at selected time intervals
fprintf('iteration number is %i \n',iter)
%disp('transient temperatures are')
fprintf('%9.3f\n',te)
plotte=[plotte te'];

iwrite=0;
end %this end goes with if iwrite>mwrite
iwrite=iwrite+1;
end %this end goes with time loop while t<tstop%%%%%%%%%%%%%%%%%%(1)
%plot the result x.vs.te by calling function figure1
subplot(1,2,1)
figure1(n,x,plotte);
%exact solution at steady-state
vx=u(1);
tl=0.03;
k0=0.1;
wa0=0.03;
pe=vx*tl/tk(1,1);
for i=1:np2
    xc(i)=0.5*(x(i)+x(i+1));
end
for i=1:np2
    c(i)=1+(1-k0)/k0*exp(pe*(xc(i)/tl-1));
    c(i)=c(i)*wa0;
end
subplot(1,2,2)
plot(xc,plotte(:,end),'--',xc,c,'x')
legend('numerical','exact')
Figure 10 Transient dopant concentration distribution in the melt (left) and comparison of steady state concentration with exact solution (right)

**Problems**

1. Derive Eq.(6)
2. Derive Eq.(21)
3. Derive Eq.(54)
4. Derive Eq.(76)

5. Derive Eq.(93)

6. A 2mm-thick plastic heat shield, initially at 0°C, is exposed simultaneously to a heat flux of 200 kW/m² from a radiation source and to a dust blast that erodes the surface at a rate of 0.1 mm/s. Calculate the temperature response of the shield. Assume following properties for plastic: \( \rho = 1200 \text{ kg/m}^3 \), \( k=0.3 \text{ W/m.K} \), and \( \alpha =0.015\times10^{-6} \text{ m}^2/\text{s} \).

7. Transpiration cooling is a process in which cold fluid is injected through a porous solid material whose outer surface is subject to a severe thermal environment. Consider a protective clothing used by a firefighter using this cooling process. The clothing is 4 mm-thickness made of material with conductivity \( k=0.2 \text{ W/m.K} \). Air (25°C) is blown through the material at 1.0 m/s. The outer surface of the clothing is subject to a black body radiation environment at 700°C. Calculate the steady state temperature distribution in the air and the clothing. (Note that \( C_p \) is constant in the air and through the clothing but conductivities in the air and clothing are different.)

8. Reconsider the experimental laser heating study discussed in Example 9.3. Suppose now the surface of the stainless steel component is exposed to a convective and radiative boundary condition as opposed to insulation. The surrounding air is at 298 K and heat transfer coefficient is 10 W/m² K. Assume the diameter of the stainless steel element is 0.5 cm. Determine the
temperature distribution and the laser beam intensity for a steady state operation. The surface emissivity of the stainless steel is 0.3.

9. Reconsider the Bridgeman process as discussed in Example 9.4 with various pulling speeds ranging from 1.0 cm/hr to 15 cm/hr. Plot the steady state concentration of dopant distribution in the melt.