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2D Advection + Diffusion Finite Element analysis

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Contents

1 Problem. Advection diffusion equation

1.1 Assumptions

To calculate concentration distribution of a material in a square area some assumption considered.

- Steady state
- 2D dimension
- Properties are constant including mass transfer coefficient
- Constant velocity
- Boundary conditions

$$
@(x,y)\begin{cases} x = 0; & c = c_0 \\ y = 0; & c = 0.01 \\ y = 1; & c = 0.01 \\ x = 1; & c = \frac{c_0}{2} \end{cases}
$$

1.2 2D advection-diffusion equation

$$
u_x \frac{\partial c}{\partial x} + u_y \frac{\partial c}{\partial y} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)
$$

$$
I = \oiint w\left[u_x \frac{\partial c}{\partial x} + u_y \frac{\partial c}{\partial y}\right] dxdy - \oiint w\left[D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)\right] dxdy = 0 \ (1)
$$

$$
\left\{
\begin{aligned}
&\oiint u_x w \frac{\partial c}{\partial x} dxdy = u_x \oint cwdy - u_x \iint \frac{\partial w}{\partial x}\frac{\partial c}{\partial x} dxdy = \cdots = u_x[-\iint \frac{\partial w}{\partial x}\frac{\partial c}{\partial x} dxdy + \oint \left[w\frac{\partial c}{\partial x}\right] n_x d\Gamma \\
&\oiint u_y w \frac{\partial c}{\partial y} dxdy = u_y \oint cwdx - u_y \iint \frac{\partial w}{\partial y}\frac{\partial c}{\partial y} dxdy = \cdots = u_y[-\iint \frac{\partial w}{\partial y}\frac{\partial c}{\partial y} dxdy + \oint \left[w\frac{\partial c}{\partial y}\right] n_y d\Gamma \\
&\oiint w\left[D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)\right] dxdy = -\iint D\left[\frac{\partial w}{\partial x}\frac{\partial c}{\partial x} + \frac{\partial w}{\partial y}\frac{\partial c}{\partial y}\right] dxdy + \oint w\left[\frac{\partial c}{\partial x} n_x + \frac{\partial c}{\partial y} n_y\right] d\Gamma = -\iint D\left[\frac{\partial w}{\partial x}\frac{\partial c}{\partial x} + \frac{\partial w}{\partial y}\frac{\partial c}{\partial y}\right] dxdy + \oint w\left[\frac{\partial c}{\partial n}\right] d\Gamma
\end{aligned}
\right.
$$

$$
\xrightarrow[\text{Green theorem}]{\text{Implementing in (1)}} \quad I = -\oiint \left[u_x \frac{\partial w}{\partial x}\frac{\partial c}{\partial x} + u_y \frac{\partial w}{\partial y}\frac{\partial c}{\partial y}\right] dxdy + \iint D\left[\frac{\partial w}{\partial x}\frac{\partial c}{\partial x} + \frac{\partial w}{\partial y}\frac{\partial c}{\partial y}\right] dxdy = 0 \quad \text{(2) weak form}
$$

Assumptions For c and w

$$
\frac{\partial w_1}{\partial x} = -\frac{1}{4bc}(c-y),\ \frac{\partial w_1}{\partial y} = \frac{1}{4bc}(b-x),\ \frac{\partial w_2}{\partial x} = \frac{1}{4bc}(c-y),\ \frac{\partial w_2}{\partial y} = -\frac{1}{4bc}(b+x),\ \frac{\partial w_3}{\partial x} = \frac{1}{4bc}(c+y),
$$

$$
\frac{\partial w_3}{\partial y} = \frac{1}{4bc}(b+x),\ \frac{\partial w_4}{\partial x} = -\frac{1}{4bc}(c+y),\ \frac{\partial w_4}{\partial y} = \frac{1}{4bc}(b-x)
$$

Then, eq. (2) can be shorted in this form of Matrixes:

$$I = -\oiint \left[u_x \begin{vmatrix} \frac{\partial w_1}{\partial x} \\ \frac{\partial w_2}{\partial x} \\ \frac{\partial w_3}{\partial x} \\ \frac{\partial w_4}{\partial x} \end{vmatrix} \begin{vmatrix} \frac{\partial c_1}{\partial x} & \frac{\partial c_2}{\partial x} \frac{\partial c_3}{\partial x} \frac{\partial c_4}{\partial x} \end{vmatrix} + u_y \begin{vmatrix} \frac{\partial w_1}{\partial y} \\ \frac{\partial w_2}{\partial y} \\ \frac{\partial w_3}{\partial y} \\ \frac{\partial w_4}{\partial y} \end{vmatrix} \begin{vmatrix} \frac{\partial c_1}{\partial y} & \frac{\partial c_2}{\partial y} \frac{\partial c_3}{\partial y} \frac{\partial c_4}{\partial y} \end{vmatrix} \right] dxdy$$

$$+ \iint D \left[\begin{vmatrix} \frac{\partial w_1}{\partial x} \\ \frac{\partial w_2}{\partial x} \\ \frac{\partial w_3}{\partial x} \\ \frac{\partial w_4}{\partial x} \end{vmatrix} \begin{vmatrix} \frac{\partial c_1}{\partial x} & \frac{\partial c_2}{\partial x} \frac{\partial c_3}{\partial x} \frac{\partial c_4}{\partial x} \end{vmatrix} + \begin{vmatrix} \frac{\partial w_1}{\partial y} \\ \frac{\partial w_2}{\partial y} \\ \frac{\partial w_3}{\partial y} \\ \frac{\partial w_4}{\partial y} \end{vmatrix} \begin{vmatrix} \frac{\partial c_1}{\partial y} & \frac{\partial c_2}{\partial y} \frac{\partial c_3}{\partial y} \frac{\partial c_4}{\partial y} \end{vmatrix} \right] dxdy$$

$$= \sum_{i=0}^{nodes} \sum u_x \breve{w}_x \check{c} + u_y \breve{w_y} \check{c} + D \sum_{i=0}^{nodes} \sum \breve{w}_x \check{c} + \breve{w_y} \check{c} = 0$$

So, this equation shall be validated by each element. For calculation, MATLAB is used.

$$\left| -u_x \begin{pmatrix} \breve{w}_{x_1}^{\ element 1^{st}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \breve{w}_{x_n}^{\ element\ n^{th}} \end{pmatrix} - u_y \begin{pmatrix} \breve{w}_{y_1}^{\ element 1^{st}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \breve{w}_{y_n}^{\ element\ n^{th}} \end{pmatrix} + D \begin{pmatrix} \breve{w}_{x_1}^{\ element 1^{st}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \breve{w}_{x_n}^{\ element\ n^{th}} \end{pmatrix} + D \begin{pmatrix} \breve{w}_{y_1}^{\ element 1^{st}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \breve{w}_{y_n}^{\ element\ n^{th}} \end{pmatrix} \right| \begin{vmatrix} c_1^{element 1^{st}} \\ \vdots \\ c_n^{element\ n^{th}} \end{vmatrix} = \begin{vmatrix} 0 \\ \vdots \\ 0 \end{vmatrix}$$

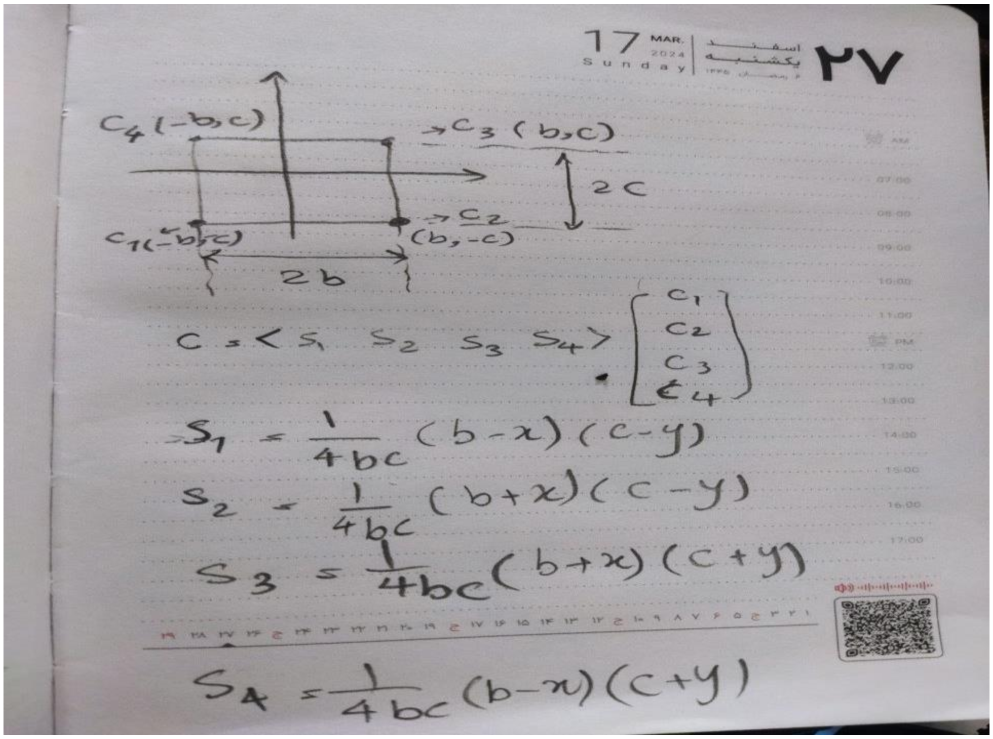
Briefly, due to simplification of boundary, the overall equation is written in this form:

$$I = \breve{w}_{global} \check{C} = 0$$

Where $\breve{w}_{global}$ $is\ a\ Matrix\ from\ acculumation\ of\ local\ matrix\ of\ elements$;

$$\breve{w}_{golbal}{}_{4*4}^{element\ n^{th}} = \begin{vmatrix} -\frac{(u_x - D)b^2 + (u_y - D)c^2}{3bc} & -\frac{(u_x - D)b^2 - 2(u_y - D)c^2}{6bc} & \frac{(u_x - D)b^2 + (u_y - D)c^2}{6bc} & -\frac{(u_x - D)c^2 - 2(u_y - D)b^2}{6bc} \\ -\frac{(u_x - D)b^2 - 2(u_y - D)c^2}{6bc} & -\frac{(u_x - D)b^2 + (u_y - D)c^2}{3bc} & -\frac{(u_x - D)c^2 - 2(u_y - D)b^2}{6bc} & \frac{(u_x - D)b^2 + (u_y - D)c^2}{6bc} \\ \frac{(u_x - D)b^2 + (u_y - D)c^2}{6bc} & -\frac{(u_x - D)c^2 - 2(u_y - D)b^2}{6bc} & -\frac{(u_x - D)b^2 + (u_y - D)c^2}{3bc} & -\frac{(u_x - D)b^2 - 2(u_y - D)c^2}{6bc} \\ -\frac{(u_x - D)c^2 - 2(u_y - D)b^2}{6bc} & \frac{(u_x - D)b^2 + (u_y - D)c^2}{6bc} & -\frac{(u_x - D)b^2 - 2(u_y - D)c^2}{6bc} & -\frac{(u_x - D)b^2 + (u_y - D)c^2}{3bc} \end{vmatrix}$$

For calculating each element concentration this formula is considered, 2nd order:



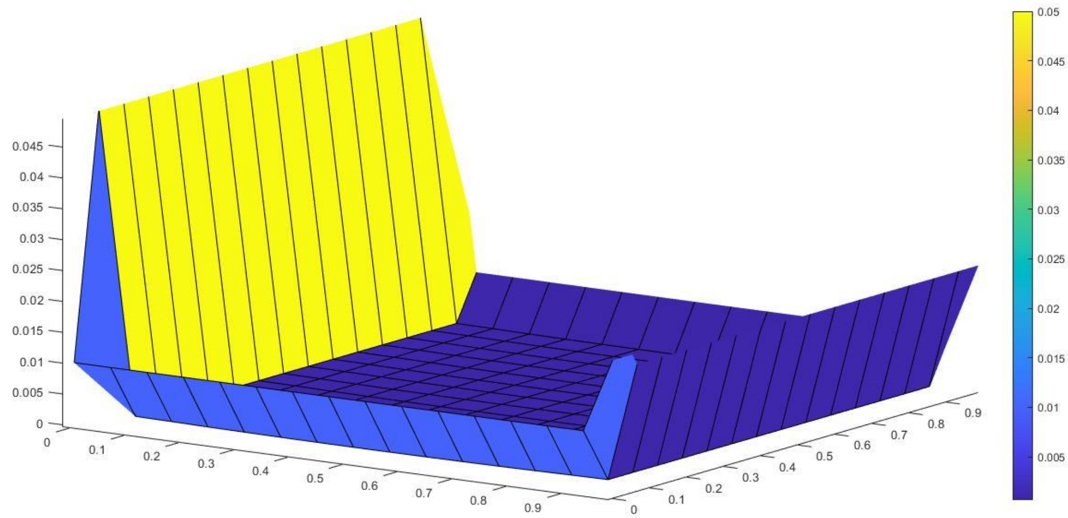
2 Solution

Following steps is considered in this work:

- Collect Mesh Information
  In this work, Quadrilateral method is applied.
- Connectivity information
  The area is continuous and solid. Consist of R^2
- Coordinate information
  xy-coordination , without any transformation, is applied.
- Boundary information
  All of boundary were considered in Dirichlet boundary.
- Look over all elements
  All of calculation was performed by MATLAB.
- Solve system of algebraic equations
  While loop with tolerance <0.0001 considered until numerical calculation converged.
- Visualize the result

3 Result

The result of calculation is depicted in a 3D-plot figure. Overall, about validations of result cannot be confirmed as the concentration distribution is not logical. The solution shows 7 steps



from governing equation to manifesting the result. The real challenge of this is that resources about applying FEM for mass transfer problem is quite rare or is not accessible in Iran.
Complexity of solution can be elaborated by adding Neumann or Robin boundary condition- in equation shall be interfaced, unsteady state- finite difference methods for calculating changes in time, triangulation, more realistic frame, distributed velocity- in this case fluid velocity equations shall be solved simultaneously, Gauss, physical properties and etc.
Regarding concentration, inner nodes are calculated roughly zero, even though initial guess was 1.0 for each node.

Notes:

1- The figure is not logical, however it could be better if mesh size was finer.

4 Code of MATLAB

```
clc
 close all
 clear all
%  An Advection and diffusion equation is solved by this code
% u_x  ?c/?x+u_y  ?c/?y=D((?^2 c)/(?x^2 )+(?^2 c)/(?y^2 ))
% Quadrilateral method

%% enter the number of element in each side ( square shape is considered)
 N1=input('enter number of elements in each row');

 N=power(N1,2);
 %% the number of nodes is calculated
 node_num=power(N1+1,2);

 %% elem matrix is the definition of each element according to it's nodes
 elem=ones(N,4);
 dx=1/N1;
 for i=1:N
     for j=1:4
         if j==1
             if mod(i,N1)==0
                 elem(i,j)=floor(i/(N1))+i-1;
             else
                 elem(i,j)=floor(i/(N1))+i;
             end
         elseif j==2
             elem(i,j)=elem(i,j-1)+1;
         elseif j==3
             elem(i,j)=elem(i,j-1)+N1;
         else
             elem(i,j)=elem(i,j-1)+1;
         end
     end
 end
 %% node matrix is the location of each element according to the xy-
coordination
 node=zeros(node_num,2);

  for i=1:node_num
     for j=1:2
         if j==1
             if mod(i,N1+1)==0
                 node(i,j)=1;
             else
                 node(i,j)=(mod(i,(N1+1))-1)*1/N1;
             end
         elseif j==2
             if mod(i,N1+1)==0
                 node(i,j)=(floor(i/(N1+1))-1)*1/N1;
             else
                 node(i,j)=floor(i/(N1+1))*1/N1;
             end
```

```
          end
      end
  end
%%  bdFlag matrix is the state of boundary condition each element;
% _ 0 for non-boundary sides;
% _ 1 for the first type, i.e., Dirichlet boundary;
% _ 2 for the second type, i.e., Neumann boundary;
% _ 3 for the third type, i.e., Robin boundary
  bdFlag=zeros(N1+1,4);
 for i=1:N
     for j=1:4
         if j==1
             if i/(N1)<=1
                 bdFlag(i,j)=1;
             end
         elseif j==2
             if mod(i,N1)==0
                 bdFlag(i,j)=1;
             end
         elseif j==3
                 if i/(N1)>N1-1
                 bdFlag(i,j)=1;
                 end
         else
             if mod(i,N1)==1
                  bdFlag(i,j)=1;
             end

         end
     end
  end

% % %  Calculation
% constants
D= 8*10^-5;   %mass transfer coeficient
u_x=10;     %x-vector of velocity
u_y=10;      %y-vector of velocity
c0= .05;       % saturated concentration in Dirichlet boundary

% %  matrix of global weight

% % % % % % Matrix of local weight

b=dx/2;
c=dx/2;
w44=zeros(4,4);

    for i=1:4
        w44(i,i)=-((u_x-D)*b^2+(u_y-D)*c^2)/(3*b*c);
    end
    w44(1,2)=-((u_x-D)*b^2-2*(u_y-D)*c^2)/(6*b*c);
    w44(1,3)=((u_x-D)*b^2+(u_y-D)*c^2)/(6*b*c);
    w44(1,4)= -((u_x-D)*c^2-2*(u_y-D)*b^2)/(6*b*c);
    w44(3,4)=w44(1,2);
    w44(2,3)=w44(1,4);
    w44(2,4)=w44(1,3);
    w44=w44+triu(w44,1)';
```

```
% % % % % % Matrix of global wieght
wglobe=zeros(node_num);
for i=1:node_num-3
    for j=1:4
        for k=1:4
        wglobe(i+j-1,i+k-1)=wglobe(i+j-1,i+k-1)+w44(j,k);
        end
    end
end

%% Matrix of Concentration
C=ones(node_num,1);
[a,b]=find(node(:,1)==0);
[aa,bb]=find(node(:,2)==0);
[aaa,bbb]=find(node(:,2)==1);
[aaaa,bbbb]=find(node(:,1)==1);
for i=a
    C(i,1)=c0;
end

for i=aa
    C(i,1)=.01;
end
for i=aaa
    C(i,1)=.01500;
end
for i=aaaa
    C(i,1)=c0/2;
end
 node1=node;
 for i=1: length(a)
wglobe(:,a(i))=0;
    wglobe(a(i),:)=0;
    wglobe(a(i),a(i))=1;
    wglobe(:,aa(i))=0;
    wglobe(aa(i),:)=0;
    wglobe(aa(i),aa(i))=1;
    wglobe(:,aaa(i))=0;
    wglobe(aaa(i),:)=0;
    wglobe(aaa(i),aaa(i))=1;
    wglobe(:,aaaa(i))=0;
    wglobe(aaaa(i),:)=0;
    wglobe(aaaa(i),aaaa(i))=1;
 end

 %% slover
CC=linsolve(wglobe,C);


%% Calculation for concentration of elements
AAA = [a; aa;aaa;aaaa];
AAA=unique(AAA);
A(:,1)=1:node_num;
AA=setdiff(A,AAA);

C_elem=zeros(N,1);
```

```
error=2;
Tol=0.0001;
counter=0;
 C1=C;
while sum(abs(error))>Tol
CC=linsolve(wglobe,C1);

for i=1:N
    S(i,1)=1/(4*b*c)*(b-node(elem(i,1),1))*(c-node(elem(i,1),2));
    S(i,2)=1/(4*b*c)*(b+node(elem(i,2),1))*(c-node(elem(i,2),2));
    S(i,3)=1/(4*b*c)*(b+node(elem(i,3),1))*(c+node(elem(i,3),2));
    S(i,4)=1/(4*b*c)*(b-node(elem(i,4),1))*(c+node(elem(i,4),2));
    C_elem(i,1)=S(i,:)*[CC(elem(i,1)); CC(elem(i,2)); CC(elem(i,3));
CC(elem(i,4))];
end


for i=1:length(AA)

        [tt,b]=find(elem(:,:)==AA(i));
for j=1:length(tt)
    C1(AA(i),1)=CC(AA(i),1)+1/length(tt)*C_elem(j,1);

end
end
error=C1-CC;

counter=counter+1;
end

%% Printing figures
%%3D figure
for i=1:N1+1
    C1(1:N1+1,i)=C1((i-1)*(N1+1)+1:(i-1)*(N1+1)+N1+1,1);


end
C1(N1+2:node_num,:)=[];
figure(1)
hold on
[X,Y] = meshgrid(0:1/(N1):1);
surf(Y,X,C1)

hold off
```