1 Methods

$$\int_{S} \rho \overline{u} \phi \cdot \overline{n} dS = \int_{S} \Gamma \frac{\partial \phi}{\partial x} \cdot \overline{n} dS + \int_{V} q_{\phi} dV \tag{1}$$

We can approximate the two surface integrals as follows:

$$\int\limits_{S} \rho \overline{u} \phi \cdot \overline{n} dS = \left(\rho \underline{(u)} S \phi \right)_{i+1} - \left(\rho \underline{(u)} S \phi \right)_{i-1} \,,$$

and

$$\int\limits_{S} \Gamma \frac{\partial \phi}{\partial x} \cdot \overline{n} dS = \left(\Gamma S \frac{\partial \phi}{\partial x} \right)_{i+1} - \left(\Gamma S \frac{\partial \phi}{\partial x} \right)_{i-1} .$$

We can approximate the volume integral as follows:

$$\int\limits_{V} q_{\phi} dV = \overline{q}V \ .$$

If we assume S is constant our transport equation becomes:

$$\left(\rho(u)\phi\right)_{i+1} - \left(\rho(u)\phi\right)_{i-1} = \left(\Gamma\frac{\partial\phi}{\partial x}\right)_{i+1} - \left(\Gamma\frac{\partial\phi}{\partial x}\right)_{i-1} + \overline{q}V.$$

We can apply the Central Differencing Scheme approximations:

$$\phi_{i+1} = \frac{\phi_{I+1} + \phi_I}{2} \qquad \qquad \phi_{i-1} = \frac{\phi_{I-1} + \phi_I}{2}$$

$$\left(\frac{\partial \phi}{\partial x}\right)_{i+1} = \frac{\phi_{I+1} - \phi_I}{\delta x} \qquad \qquad \left(\frac{\partial \phi}{\partial x}\right)_{i-1} = \frac{\phi_I - \phi_{I-1}}{\delta x}$$

The transport equation now looks like:

$$\left(\frac{\rho \overline{u}}{2}\right)_{i+1} \left(\phi_{I+1} + \phi_I\right) - \left(\frac{\rho \overline{u}}{2}\right)_{i-1} \left(\phi_{I-1} + \phi_I\right) = \frac{\Gamma}{\Delta x} \left(\phi_{I+1} - \phi_I\right) - \frac{\Gamma}{\Delta x} \left(\phi_I - \phi_{I-1}\right) + \overline{q}_I \Delta x.$$

For this problem, the density and velocity are constant throughout the geometry. We can group terms and get the transport equation in a useful form to sovle.

$$\left[-\frac{\rho \overline{u}}{2} - \frac{\Gamma}{\Delta x} \right] \phi_{I-1} + \left[\frac{2\Gamma}{\Delta x} \right] \phi_I + \left[\frac{\rho \overline{u}}{2} - \frac{\Gamma}{\Delta x} \right] \phi_{I+1} = \overline{q}_I \, \Delta x \tag{2}$$

We can rewrite this equation as:

$$a_I \phi_{I-1} + b_I \phi_I + c_I \phi_{I+1} = Q_I . (3)$$

This equation works for middle nodes, but the edge nodes do not have enough neighbor nodes. The first node does not have another node to the left of it (I-1), so we have to only use the value at the left edge, which is ϕ_L . This gives us:

$$\left[\left(\frac{\rho \overline{u}}{2} \right)_{i+1} + \frac{3\Gamma}{\Delta x} \right] \phi_I + \left[\left(\frac{\rho \overline{u}}{2} \right)_{i+1} - \frac{\Gamma}{\Delta x} \right] \phi_{I+1} = \overline{q}_I \, \Delta x + (\rho \overline{u} \phi)_L + \frac{2\Gamma}{\Delta x} \phi_L \,, \tag{4}$$

which gives us an equation of the form:

$$b_1 \phi_1 + c_1 \phi_2 = Q_1 \ . \tag{5}$$

If we do the same on the right side we get:

$$\left[-\left(\frac{\rho \overline{u}}{2}\right)_{i-1} + \frac{3\Gamma}{\Delta x} \right] \phi_{I-1} + \left[-\left(\frac{\rho \overline{u}}{2}\right)_{i-1} - \frac{\Gamma}{\Delta x} \right] \phi_{I} = \overline{q}_{I} \, \Delta x - (\rho \overline{u}\phi)_{R} + \frac{2\Gamma}{\Delta x}\phi_{R} \,, \tag{6}$$

and:

$$a_N \phi_{N-1} + b_N \phi_N = Q_N . (7)$$

2 Results

Figure 1 shows the two solutions for Case 1: 5 control volumes and $\overline{u} = 0.1 \,\mathrm{m\,s^{-1}}$. Figure 2 shows the two solutions for Case 2: 5 control volumes and $\overline{u} = 2.5 \,\mathrm{m\,s^{-1}}$. Figure 3 shows the two solutions for Case 3: 20 control volumes and $\overline{u} = 2.5 \,\mathrm{m\,s^{-1}}$.

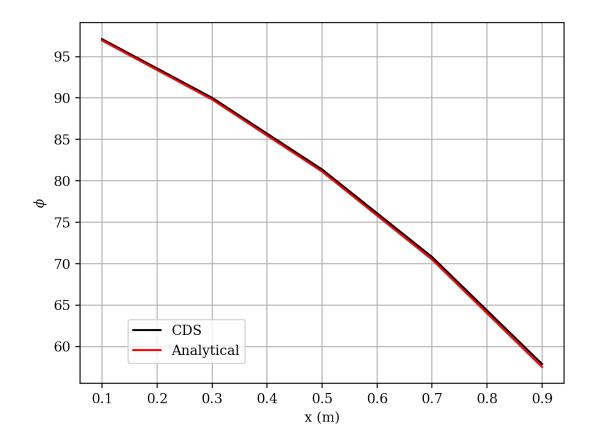


Figure 1: Central Difference Scheme and Analytical Solutions for Case 1.

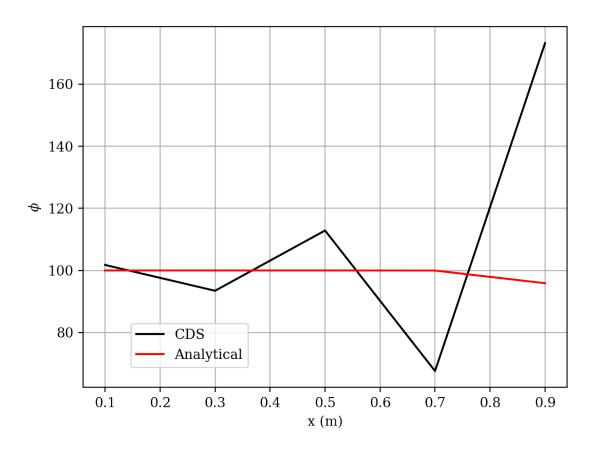


Figure 2: Central Difference Scheme and Analytical Solutions for Case 2.

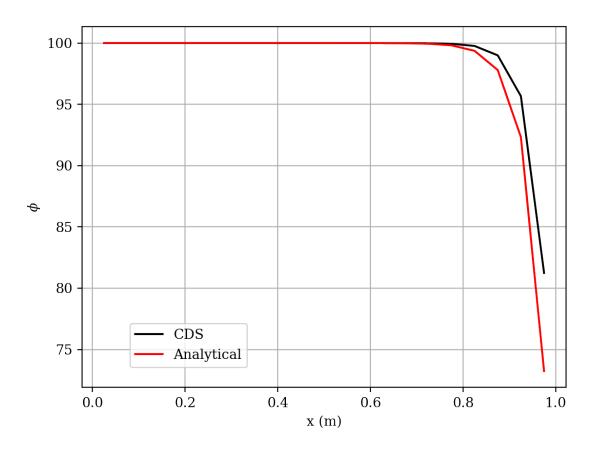


Figure 3: Central Difference Scheme and Analytical Solutions for Case 3.

Table 1 lists the error values calculated for each case.

Table 1: Error values for each case.

Case	Error
1	0.2629491288831474
2	26.174593696190538
3	0.6567406338821179

3 Discussion

We can use the Peclet number to see how stable each solution should be to determine if the solutions perform how we expect them to.

$$Pe = \frac{\rho \overline{u}}{\Gamma/\Delta x} \tag{8}$$

For this problem, we want Pe < 2. Table 2 shows the Peclet numbers for each case. As we can see, the second case does not meet the criteria for stability, so we expect the numerical solution to be unstable. The other two solutions are expected to be stable and they are. Also, the solutions go from a value of 100 on the left towards a value of 50 on the right, which we would expect from the boundary conditions.

Table 2: Peclet number for each case.

Case	Pe
1	0.2000000000000000004
2	5.0
3	1.25

4 Code

```
10 # define central difference scheme function to use for each case
def cds_ss(num_volumes, tot_length, velocity, density, diffusion,
       source, left, right):
       """Function to perform central difference scheme to solve one
12
          -dimensional steady state transport with convection and
          diffusion.
13
14
       Parameters
15
       num_volumes : float
16
           The number of discretized volumes.
17
18
       tot_length : float
           The total length of the pipe in meters.
19
       velocity : float
20
           The average velocity of the flow in meters per second.
21
22
       density : float
           The density of the flow in kilograms per cubic meter.
23
24
       diffusion : float
25
           The diffusion coefficient in kilogram-seconds per meter.
       source : float
26
           The source term in [units].
27
       left : float
28
           The left boundary condition.
29
       right : float
30
           The right boundary condition.
31
32
33
       Returns
34
       phi : numpy.ndarray
35
           Solved flux profile.
36
37
       dx = tot_length/num_volumes
38
       phi = np.zeros(num_volumes)
39
       A = np.zeros((num_volumes,num_volumes))
40
       Q = np.zeros(num_volumes)
41
42
43
44
45
       for j in range(num_volumes):
46
           if j == 0:
47
               A[j,0] = density*velocity/2 + 3*diffusion/dx
48
               A[j,1] = density*velocity/2 - diffusion/dx
49
               Q[j] = density*velocity*left + 2*diffusion*left/dx
50
51
```

```
elif j == num_volumes-1:
52
                A[j,j-1] = -density*velocity/2 - diffusion/dx
53
                A[j,j] = -density*velocity/2 + 3*diffusion/dx
54
                Q[j] = -density*velocity*right + 2*diffusion*right/dx
55
56
           else:
57
                A[j,j-1] = -\text{density} * \text{velocity}/2 - \text{diffusion}/\text{dx}
58
                A[j,j] = 2*diffusion/dx
59
                A[j,j+1] = density*velocity/2 - diffusion/dx
60
                Q[j] = 0
61
62
63
       phi = np.linalg.solve(A,Q)
       return phi
64
65
66
67
68 # define analytical solution function to use for each case
   def analytical(num_volumes, tot_length, velocity, density,
      diffusion, left, right):
       """Function to analytically solve one-dimensional steady
70
          state transport with convection and diffusion.
71
72
       Parameters
73
74
       num_volumes : float
           The number of discretized volumes.
75
       tot_length : float
76
           The total length of the pipe in meters.
77
       velocity : float
78
           The average velocity of the flow in meters per second.
79
       density : float
80
            The density of the flow in kilograms per cubic meter.
81
82
       diffusion : float
           The diffusion coefficient in kilogram-seconds per meter.
83
       left : float
84
           The left boundary condition.
85
       right : float
86
           The right boundary condition.
87
88
89
       Returns
90
       phi : numpy.ndarray
91
           Solved flux profile.
92
93
94
       dx = tot_length / num_volumes
```

```
x = np.linspace(dx/2, tot_length-(dx/2), num=num_volumes,
95
           endpoint=True)
        phi = left + (right-left) * (np.exp(density*velocity*x/
96
          diffusion)-1)/(np.exp(density*velocity*tot_length/
          diffusion)-1)
        return phi
97
98
99
100
101
102
   def error_calc(phi_exact, phi):
        """Function to calculate error.
103
104
105
       Parameters
106
        phi_exact : numpy.ndarray
107
            The exact solution.
108
       phi : numpy.ndarray
109
110
            The approximate solution.
111
112
        Returns
113
114
        error : float
            The average error for the approximate solution.
115
116
117
        error = np.sum(np.abs(phi_exact - phi)) / len(phi)
118
        return error
119
120
121 # define constants
122 tot_length = 1 # pipe length in meters
123 density = 1 # density in kg/m^3
124 diffusion = 0.1 # diffusion coefficient in kg-s/m
125 source = 0
                   # source
126 	 left = 100
                   # left hand boundary condition
127 right = 50 # right hand boundary condition
128
129 # define variables
130 velocity = np.array([0.1, 2.5, 2.5])
131 num_volumes = np.array([5,5,20])
132 Pe = np.zeros(len(velocity))
133
134
135 error = np.zeros(len(velocity))
136 # solve
```

```
for k in range(len(velocity)):
137
        phi = cds_ss(num_volumes[k], tot_length, velocity[k], density
138
           , diffusion, source, left, right)
        phi_exact = analytical(num_volumes[k], tot_length, velocity[k
139
          ], density, diffusion, left, right)
        error[k] = error_calc(phi_exact,phi)
140
        dx = tot_length / num_volumes[k]
141
        Pe[k] = density * velocity[k] * dx / diffusion
142
143
144
145
        x = np.linspace(dx/2, tot_length-(dx/2), num=num_volumes[k])
146
147
        plt.rcParams['font.family'] = 'serif'
        plt.rcParams['mathtext.fontset'] = 'dejavuserif'
148
        plt.figure(facecolor='w', edgecolor='k', dpi=200)
149
        plt.plot(x, phi, '-k', label='CDS')
150
        plt.plot(x, phi_exact, '-r', label='Analytical')
151
        plt.xlabel('x (m)')
152
153
        plt.ylabel(r'$\phi$')
        plt.figlegend(loc='right', bbox_to_anchor=(0.4,0.2))
154
       plt.grid(b=True, which='major', axis='both')
155
        plt.savefig('HW1/plots/graph_case'+str(k+1)+'.png',
156
           transparent=True)
        plt.savefig('HW1/plots/graph_case'+str(k+1)+'.svg',
157
           transparent=True)
158
159
160
   # generate latex table for error
161
   out_file = open('HW1/tabs/error_tab.tex','w')
162
   out_file.write(
163
                    '\\begin{table}[htbp]\n'+
164
165
                    '\t \centering\n'+
                    '\t \caption{Error values for each case.}\n'+
166
167
                    '\t \\begin{tabular}{cc}\n'+
                    '\t\t \\toprule\n'+
168
                    '\t\t Case & Error \\\ \n'+
169
                    '\t\t \midrule \n'+
170
171
                    '\t\t 1 & '+str(error[0])+' \\\ \n'+
                    '\t\t 2 & '+str(error[1])+' \\\ \n'+
172
                    '\t\t 3 & '+str(error[2])+' \\\ \n'+
173
                    '\t\t \\bottomrule \n'+
174
175
                    '\t \end{tabular} \n'+
                    '\t \label{tab:error} \n'+
176
                    '\end{table}'
177
```

```
178 )
179
180
181 # generate latex table for Peclet numbers
   out_file = open('HW1/tabs/Pe_tab.tex','w')
   out_file.write(
183
                     '\\begin{table}[htbp]\n'+
184
185
                     '\t \centering\n'+
                     '\t \caption{Peclet number for each case.}\n'+
186
                     '\t \\begin{tabular}{cc}\n'+
187
                     '\t\t \\toprule\n'+
188
                     '\t\t Case & $Pe$ \\\ \n'+
189
                     '\t\t \midrule \n'+
190
                     '\t\t 1 & '+str(Pe[0])+' \\\ \n'+
191
                     '\t\t 2 & '+str(Pe[1])+' \\\ \n'+
192
193
                     '\t\t 3 & '+str(Pe[2])+' \\\ \n'+
                     '\t\t \\bottomrule \n'+
194
195
                     '\t \end{tabular} \n'+
196
                     '\t \label{tab:Pe} \n'+
                     '\end{table}'
197
198
   )
```