Diploma Work

Numerical simulation of steady and unsteady mass transfer over a two-dimensional electrochemical sensor

By:
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Summary

A mass transfer probe is a device to measure the wall shear stress in a liquid flow. A chemical reaction, a mass transfer, is carried out on the surface of the probe and is proportional to the current arising in the electrode circuit. The measured current is related to the velocity gradient $S$, at the surface of the probe. If the viscosity $\eta$ of the liquid is known the wall shear stress $\sigma_w=\eta S$ can consequently be calculated.

For a rectangular mass transfer probe, a series of assumptions regarding the geometry and flow properties let the mass balance equation over the probes surface be written in the simplified two-dimensional form Eq. (1). The mass transfer Eq. (2) is calculated from an integration of the concentration gradient at the surface along the probe. (expressed in non dimensional units designated by $\ast$):

$$\frac{\partial C^+}{\partial t^+} + S^+ y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^+ \partial x^+} + \frac{\partial^2 C^+}{\partial x^+ \partial y^+} \quad (1),$$

$$K^+=L_p \int \frac{\partial C^+}{\partial y^+} \bigg|_{y^+}^{y^+=0} \, dx^+ \quad (2)$$

Defining boundary conditions and introducing an input signal, a velocity gradient $S^+$, a relation between $S^+$ and $K^+$ have been obtained previously by other authors by solving Eqs. (1) and (2). This relation can be used to translate an experimental measured mass transfer $K^+$ to a velocity gradient $S^+$, and consequently a wall shear stress $\sigma_w=\eta S$. In previous studies it has been assumed that for high rate of convection $S^+>5000$ the x-diffusion term $\frac{\partial^2 C^+}{\partial x^+ \partial y^+}$ can be neglected.

In this study, computer programs that solve the steady ($\frac{\partial C^+}{\partial t^+}=0$) and unsteady mass balance equation over a rectangular mass transfer probe have been developed. The finite volume method has been used to discretise the mass balance equation to algebraic relations and the computer codes have been made with Matlab. Comparisons with analytical solutions and grid independence studies have been conducted that validate the codes.

Numerical simulations of the steady mass balance equation for a large range of constant input signals $S^+$ have been conducted and the corresponding mass transfers $K^+$ have been computed. A good agreement with previous studies was found. A study of the effect on $K^+$ of neglecting the x-diffusion has been conducted and it has been concluded that a neglecting the x-diffusion gives a maximum error of 1.4 % for values of $S^+>5000$.

The frequency response of the mass transfer probe has been obtained by performing numerical simulations of the unsteady mass balance equation when introducing a sinusoidal input signal, $S^+=S^+ \sin(2\pi f^+ t^+)$, with low amplitude fluctuations $\hat{s}^+<<S^+$. When neglecting the x-diffusion the frequency response agrees fairly well with previous studies. This study shows however that when taking the x-diffusion into consideration the frequency response looks different. The x-diffusion seems to have a damping and especially phase delaying effect on the mass transfer and should not be neglected, not even for input signals higher than $S^+>5000$.

Keywords: Mass transfer probe, Mass transfer, Velocity gradient, Mass balance equation, X-diffusion, Sinusoidal inputs signal, Low amplitude fluctuation, Frequency response, Damping, Phase delay.
List of symbols

C  concentration
C_B  bulk concentration
c  courant number
D  diffusion coefficient
f  frequency of s
H  height of the computational domain
K  mass transfer coefficient for the probe
\overline{K}  time average of K
k  time dependent component of the mass transfer coefficient
\dot{k}  amplitude of k
L_F  length of the upstream probe-edge (leading edge)
L_P  length of the probe
L_R  length of the downstream probe-edge (trailing edge)
< N >  molar flux of electrons
S  velocity gradient at the wall
\overline{S}  time average of S
\dot{s}  time dependent component of velocity gradient at the wall
\ddot{s}  amplitude of s
Sc  Schmidt number
Pe  Peclet number
t  time
U  streamwise velocity
W  width of the probe
x  distance in the direction of the mean flow
y  distance perpendicular to the wall

Greek Symbols

\Delta \Theta  phase delay
\Delta x  width of a control volume
\Delta y  height of a control volume
\bar{\delta}_c  thickness of the concentration boundary layer
\bar{\delta}_u  thickness of the velocity boundary layer
\iota  viscosity
\dot{i}  kinematic viscosity
\dot{\omega}_w  wall shear stress

Superscripts

+  Nondimensionalized with probe length L_p, diffusion constant D, and bulk concentration C_B
\(a_w\) coefficients representing the influence of both convection and diffusion from neighbours nodes W, E, S and N to node P

\(a_E\)

\(a_S\)

\(a_N\)

\(a_p\) central coefficient

\(D_w\) coefficients representing influence of diffusion from the west and east face of a control volume, to node P

\(D_e\)

\(F_w\) coefficients representing influence of convection from the west and east face of a control volume, to node P

\(F_e\)
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Section 1: Introduction

1.1 Previous studies

A fluid flowing past a solid boundary exerts stress to the surface of the boundary in the normal and tangential direction of the flow. To measure the pressure in the normal direction is fairly easy, for example by drilling a hole in the surface and connect to a manometer. However, a measurement of the stress in the tangential direction, the wall shear stress, is not as easily conducted, and different ways of measuring it has been discussed and carried out through the years. Some of the methods are; Stanton tube, direct measurement, hot-film sensor, the Preston tube and the electrochemical technique. Knowing the behaviour of the wall shear stress is of considerable importance since it would yield a better understanding of the fluid transport and the structure of the shear flow.

As stated above one of the methods of measuring the wall shear stress is using the electrochemical technique, or the mass transfer probe which is the term that is going to be used further on in this report. The advantages of this method are that it doesn’t interfere with the flow, it can be used in a wide variety of flows, it offers the possibility of measuring time-varying flows and that calibration is not necessary. One of the disadvantages with the mass transfer probe when compared with the hot-film sensor, is that the frequency response is not as good. Another disadvantage is that the use of mass transfer probes is limited to liquid flows.

A description of how the electrochemical method works will be stated here. The mass transfer probe is a part of an electrochemical cell as sketched in Figure 1.1. Two cells are mounted at the wall in a channel, to the left the cathode and to the right the anode which are referred to the mass transfer probe, or just the probe and the counterelectrode respectively. The flowing fluid that is to be studied consists of a reacting electrolyte. The surface of the mass transfer probe studied in this report has a rectangular shape.

![Figure 1.1 Electrochemical cell](image)

At the mass transfer probe a reduction is taken place, that is, the ions in the electrolyte receive electrons from the probe. At the counterelectrode the reverse reaction occurs. A negative voltage is applied to the mass transfer probe in order to operate it cathodically. The applied voltage is controlled so that the reaction at the mass transfer probe is polarized. I.e. the concentration of the ions that receive electrons at the mass transfer probe is approximately zero. That is, the reaction is fast and every ion in the immediate vicinity of the surface of the probe receives an electron as soon it contacts the surface (fast kinetic assumption). With the flow of electrons, a current in the electrode circuit arises, which can be measured. The current
produced in the reaction is proportional to the molar flux of electrons, or mass transfer \( <N> \) at the mass transfer probe, which is calculated by using Faraday’s law.

Let the concentration of ions in a fluid particle be denoted \( C \). The concentration at the probes surface is via the polarization kept at the value \( C=0 \). Let the concentration of a fluid particle unaffected by the probe be denoted \( C_B \) (bulk concentration). Hence, with the presence of the mass transfer probe a concentration gradient and a concentration boundary layer are developed.

The mass transfer process occurring at the electrode is characterized by large Schmidt number \((Sc=\nu/D)\). The probes have therefore the desirable feature that there is a quite large range of flow rates over which the concentration boundary layer is within a region where the velocity field can be approximated by the linear relation Eq. (1.1).

\[
U = S_y y \quad \text{(1.1)}
\]

Where \( S_y = \frac{\partial U}{\partial y} \bigg|_{y=0} \) is the velocity gradient at the wall. Reiss and Hanratty (1962) were the first ones to show how the measured current can be related to the velocity gradient at the wall. If the viscosity of the liquid is known, the wall shear stress \( \nu \frac{\partial U}{\partial y} \bigg|_{y=0} \) can consequently be calculated.

1.1.1 Translating a measured current to wall shear stress

How can then a measured current be connected to the wall shear stress? As stated above Faraday’s law is used to calculate the molar flux of electrons \( <N> \) from the current. Let a mass transfer coefficient or simply a mass transfer \( K \) be defined as \( K = \frac{<N>}{C_B} \).

The mass balance equation

A theoretical connection between the mass transfer \( K \) and the wall shear stress \( S \) can be established by solving the governing mass balance equation that describes the distribution of concentration in a concentration boundary layer.

A several assumptions have been made to simplify the general 3-dimensional mass balance equation into the simplified 2-dimensional one Eq. (1.2). The equation is expressed in terms of non dimensional units. The assumptions and the non dimensionalisation that yield the following equation will be explained in detail later in Section 2.

\[
\frac{\partial C^+}{\partial t^+} + S^+ y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^+ \partial t^+} + \frac{\partial^2 C^+}{\partial x^+ \partial y^+} \quad \text{(1.2)}
\]

The mass transfer at the probe can be written as:

\[
K^+ = L_p \int_{y^+ = 0}^{y^+} \frac{\partial C^+}{\partial y^+} \, dx^+ \quad \text{(1.3)}
\]

Let Eq. (1.2) be studied. By introducing a velocity gradient \( S^+ \) and defining valid boundary conditions, the only remaining unknown variable is the concentration \( C^+(x,y,t) \). If the concentration \( C^+ \) is calculated, also the mass transfer \( K^+ \) can be calculated by using Eq. (1.3).
This has been done previously both analytically and numerically (Mitchell Hanratty (1966), Fortuna, Hanratty (1971) and Py (1990)). Performing such studies yields a theoretical relation between $S^+$ and $K^+$. This relation makes it possible connect experiment to theory, i.e. to translate an experimentally measured mass transfer to a velocity gradient and a wall shear stress.

The results from those previous studies are obtained assuming that the streamwise diffusion term $\frac{\partial^2 C^+}{\partial x^2}$ in Eq. (1.2) can be neglected. The flows over a mass transfer probe are of high convective character and Ling (1962) showed that the term may be neglected for $S^+ > 5000$.

**Steady flow**

For a steady flow it is fairly easy to obtain a relation between $K^+$ and $S^+$ by solving the coupled Eqs. (1.2) and (1.3). When the flow is steady the velocity gradient $S^+$ is constant and the time dependent term in Eq. (1.2) is $0$. When neglecting the x-diffusion Eq. (1.2) has an analytic solution and the equation for the mass transfer, Eq. (1.3), can be written as:

$$K^+ = 0.807 S^{+1/3}$$  \hspace{1cm} (1.4)

**Fluctuating flow**

Obtaining a relation between $K^+$ and $S^+$ however, is more complicated for a fluctuating flow. In a fluctuating flow the velocity gradient $S^+$ fluctuates. Hence, the mass transfer and consequently the measured current will also fluctuate. In order to obtain a relation between $K^+$ and $S^+$ for a fluctuating flow it has of been of interest to study solutions to Eqs. (1.2) and (1.3) when introducing a sinusoidal velocity gradient $S^+$.

**Frequency response**

Let $S^+$ be defined as the sum of time average property and fluctuating property as

$$S^+ = \bar{S}^+ + s^+$$  \hspace{1cm} (1.5)

Now, defining the fluctuating property as a sinusoidal function, (1.5) reads:

$$S^+ = \bar{S}^+ + \hat{s}^+ \sin(2\pi f^+ t^+)$$  \hspace{1cm} (1.6)

Where $\hat{s}^+$ and $f^+$ are the amplitude and the frequency of fluctuating property $s^+$ respectively. It has via numerical simulations been analyzed how the mass transfer depends of and responds to different frequencies of a sinusoidal input signal Eq. (1.6). Most of the work on the frequency response of mass transfer probes has involved an assumption that the amplitude of the fluctuations is small compared to the time-average flow $\hat{s}^+ \ll \bar{S}^+$. For an input signal with small amplitude fluctuation it has been showed that the mass transfer $K^+$ varies sinusoidally with the same frequency as the input signal but with a phase delay, $\Delta \Theta$, that increases with an increasing input frequency. Furthermore, it has been showed that the amplitude of the mass transfer coefficient, $\hat{k}^+$, is damped with increasing input frequency (Mitchell Hanratty (1966)).
\[ K^+ = K^+ + \hat{k}^+ \sin(2\pi f^+ t^+ + \Delta \Theta) \]  

(1.7)

I.e. due to the inertia inherent to the system it takes some time for the probe to feel the variation of \( S^+ \). If the probe would have reacted instantaneously to the variation of \( S^+ \) the signals would be in phase (\( \Delta \Theta = 0 \)) independently of the input frequency \( f^+ \). The damping and phase delaying character is referred to as the frequency response of the probe.

1.2 Objective

Programming
The first objective of this study is to develop a computer program that numerically solves the mass balance equation Eq. (1.2) for a flow over a rectangular mass transfer probe. The finite volume method is going to be used to transform the partial differential equation to algebraic relations and the computer codes will be made in Matlab. Two codes will developed, one that solves the unsteady mass balance equation and one that solves the steady mass balance equation (\( \frac{\partial C^+}{\partial t^+} = 0 \)). Grid independence studies and comparisons with analytical solutions will be made to validate the codes.

Numerical simulations
The second objective of the study is to use the codes to perform numerical simulations of the steady and unsteady mass balance equation.

In the first part the results from numerical simulations of the steady mass balance equation will be presented and analyzed. Simulations for a large range of constant input signals \( S^+ \) will be conducted and the corresponding mass transfers \( K^+ \) will be calculated, in order to investigate how \( K^+ \) depends on \( S^+ \) in a steady flow. Further, it will be investigated how the solution and the values of \( K^+ \) change when neglecting the \( x \)-diffusion. The results are to be compared with the analytic expression stated in Eq. (1.4).

The second part the result from the numerical simulations of the unsteady mass balance equation will be presented and analyzed. Simulations for sinusoidal input signals \( S^+ \) with different frequencies will be performed to investigate the frequency response of the mass transfer probe. It will also be investigated how the frequency response changes when neglecting the \( x \)-diffusion. The result will then be compared with the frequency response reported by Py (1990).
Section 2: Physical model

2.1 Flow over a rectangular mass transfer probe

Now, consider the flow over a probe, with dimensions $L_p \times W$, as sketched in Figure 2.1 below in which an electrochemical reaction occurs at the probe surface. The mass transfer at the probe surface is denoted as $<N>$ and the concentration of the reacting species in the inflow as $C_B$. The mass transferred at the surface is only due to diffusion and is determined by an expression that is analogous to Fourier’s law. For the conditions of interest in this text, the expression, which is called Fick’s law, has the form:

$$N'' = -D \frac{\partial C}{\partial y}$$  \hspace{1cm} (2.1)

The total mass transfer at the probe can be deduced by integrating (2.1) over the total probe area.

$$<N> = D \int_{\text{probe \ area}} \frac{\partial C}{\partial y} \, dy \, dz$$  \hspace{1cm} (2.2)

A mass transfer coefficient $K$ can then be defined as:

$$K = \frac{<N>}{C_B}$$  \hspace{1cm} (2.3)

considering that the concentration of the reacting chemical specie at the probe is zero. This hypothesis is reasonable for fast chemical reactions (i.e when the characteristic time scale of the chemical reaction is much smaller than the diffusion time scale).

Figure 2.1 Flow over a probe
For a concentration boundary layer the governing mass balance equation in a three-dimensional incompressible flow field can be written as:

\[
\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial y} + W \frac{\partial C}{\partial z} = D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) \tag{2.4}
\]

\(C(x, y, z, t)\) = Concentration of reaction electrolyte [kmol/m\(^3\)]

\(U(x, y, z, t)\) = Velocity in the x-direction [m/s]

\(V(x, y, z, t)\) = Velocity in the y-direction [m/s]

\(W(x, y, z, t)\) = Velocity in the z-direction [m/s]

\(\frac{\partial C}{\partial t}\) = Rate of change of C [kmol/m\(^3\) s]

\(U_j \frac{\partial C}{\partial j}\) = Rate of change of C due to convection in the j-direction [kmol/m\(^3\) s]

\(\frac{\partial^2 C}{\partial j^2}\) = Rate of change of C due to diffusion in the j-direction [m/s]

\(D\) = Diffusion coefficient of the reacting electrolyte [m\(^2\)/s]

And the equation for the mass transfer coefficient as:

\[
K = \frac{D}{C \left[ \frac{\partial C}{\partial y} \right]_{y=0}} \int \int \frac{\partial C}{\partial y} \text{dxdz} \tag{2.5}
\]

Now, a series of assumptions will be made to simplify Eq. (2.4).

- It has been shown that if the width \(W\) of a rectangular probe is large enough (a large value of \(W/L\)), the edge effects in the transverse direction (coordinate \(z\)) are negligible. Therefore the first two derivatives of the concentration \(C/\partial z\) and \(\frac{\partial^2 C}{\partial z^2}\) can be neglected and (7) is reduced to a 2-dimensional equation.

![Figure 2.2 Velocity and concentration boundary layers](image)

- The liquid flows where mass transfer probes are used involve high Schmidt numbers, which results in that the thickness of the concentration boundary layer \(\delta_c\) is much smaller than the velocity boundary layer \(\delta_u\), as illustrated in Figure 2.2 above (i.e. the concentration boundary layer lies within the domain that in turbulence theory is referred to as the linear sublayer.)
where there is a linear relation between the velocity and the distance from the wall; 
\( U(x,y,t) = ky \) for a given \( x \) and \( t \).

- The length of the probe is very small in the x-direction (\( \approx 10^{-5} \) m) and it has therefore also been assumed that \( U \) is independent of the stream wise coordinate \( x \). The velocity \( U \) may therefore be expressed, using the velocity gradient at the wall, as:

\[
U(y, t) = S(t)y
\]  
(2.6)

\[
S(t) = \frac{\partial U}{\partial y}_{y=0} = \text{velocity gradient at the wall}
\]  
(2.7)

![Figure 2.3 Linear velocity profile](image)

By inserting Eq. (2.6) in the 2-dimensional continuity equation Eq. (2.8):

\[
\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0
\]  
(2.8)

it can be verified that since \( U \) is a function of \( y \) only, the first term in Eq. (2.8) \( \frac{\partial U}{\partial x} = 0 \). As a result \( V \) must be a constant. And because of the no slip condition, \( V=0 \) at the wall, \( V \) equals zero in the entire domain, and the term \( V \) in Eq. (2.4) can be neglected.

- Consequently the mass balance equation (2.4) can be simplified to:

\[
\frac{\partial C}{\partial t} + Sy \frac{\partial C}{\partial x} = D \left( \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial x^2} \right)
\]  
(2.9)

The following transformation in which \( L_p \) is the probe length, \( t \) the time, \( C_B \) is the bulk concentration and \( f \) the frequency of the time evolution of the velocity gradient which is assumed to have the form \( S = \tilde{S} + \ddot{S}\sin(2\pi ft) \):

- \( C^+ = \frac{C}{C_B} \)
- \( x^+ = \frac{x}{L_p} \)
- \( y^+ = \frac{y}{L_p} \)

- \( S^+ = \frac{S L_p^2}{D} \)
- \( t^+ = \frac{tD}{L_p^2} \)
- \( f^+ = \frac{fL_p^2}{D} \)

- \( K^+ = \frac{K L_p}{D} \)

renders a dimensionless form of the unsteady mass balance equation and for the mass transfer coefficient \( K \).
\[
\frac{\partial C^+}{\partial t^+} + S^+ y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^+^2} + \frac{\partial^3 C^+}{\partial x^+^2}
\]

(2.10)

\[
K^+ = L_p \int_{y^+ = 0}^{y^+ = 0} \frac{\partial C^+}{\partial y^+} \, dx^+
\]

(2.11)

By letting the time derivative, \( \frac{\partial C^+}{\partial t^+} = 0 \), the steady state mass balance equation is obtained.

\[
S^+ y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^+^2} + \frac{\partial^3 C^+}{\partial x^+^2}
\]

(2.12)

It has above been shown that by using a series of assumptions regarding the flow- and geometry properties, the governing equation for three dimensions (2.4 can be simplified to the more simple two dimensional case, eq. (2.10).

Let equation (2.10) be studied. Supposing the velocity gradient \( S^+ \), the input signal is known, and boundary conditions are well defined. The only remaining unknown variable is the concentration \( C^+ \). If the concentration \( C^+ \) is calculated, also the mass transfer \( K^+ \), the output signal can be calculated by using equation (2.11).

In the following section, the mathematical model, the boundary conditions and computational domain will be defined. The steady and unsteady mass balance equation will be discretised into algebraic relation with the finite volume method. The section also contains grid independence studies that confirms that the computational domain, grid and time steps are appropriate.
Section 3: Mathematical Model

3.1 Boundary conditions

Consider the domain $\Omega$ as sketched in Figure 3.1.

The flow is from left to right where:
- $L_F$: Length of the upstream probe-edge (leading edge)
- $L_P$: Length of probe
- $L_R$: Length of the downstream probe-edge (trailing edge)
- $H$: Height of the domain

In accordance with previous studies (Mitchell Hanratty (1966), Fortuna, Hanratty (1971) and Py (1990)) the boundary conditions are the following:

1: Inflow boundary ($x^+=0$)
   $C^+=1$ (C=$C_B$)

2: Well outside the concentration boundary layer ($y^+=H$)
   $C^+=1$ (C=$C_B$)

3: Outflow boundary ($x^+=L_F+L_P+L_R$)
   $\frac{\partial C^+}{\partial x^+} = 0$

4.6: Channel wall ($x^+<L_P$ and $x^+>L_F+L_P$)
   $\frac{\partial C^+}{\partial y^+} = 0$ (zero mass flux, impermeable surface)

5: Surface of probe ($L_F<x^+<L_F+L_P$)
   $C^+ = 0$ (fast kinetic assumption)
3.2 Numerical techniques

The governing equations are written in a Cartesian coordinate system. The finite volume method was used to transform the partial differential equations to algebraic relations. The TDMA (Tri-Diagonal matrix solver) was employed to solve the obtained algebraic relation. To approximate the convection fluxes the hybrid differencing scheme was used and the diffusion terms were discretized with central differencing for the spatial discretization and the Crank Nicolson scheme for time discretization. In making this study conventional numerical and discretization techniques were used. Further detailed information about the finite volume method and the discretization schemes (Hybrid scheme, Crank Nicolson scheme) can be found in Versteeg and Malalasekera (1995). All programming was made in Matlab and the codes are attached in appendix 5.

![Figure 3.2: The control volume finite volume grid covering the computational domain](image)

3.2.1 Mesh generation

Figure 3.2 depicts a sketch of the computational mesh. The domain is divided into non-overlapping control volumes by the lines that define the boundaries of the individual control volumes. At the center of each control volume there is a node, designated by a circle. Two sets of grid lines can be identified: the grid lines that define the control volume faces, and the grid lines (not shown) that define the locations of the nodes. In the computer implementation (the Matlab codes) the grid lines that define the node locations will be stored in the variables x_node(i,j) and y_node(i,j). The grid lines that define the control volume interfaces will be stored in x_grid(i,j) and y_grid(i,j).

Nodes in the domain may be identified by their (i,j) indices. An additional naming convention based on the directions on a map will be used to simplify the algebra in the following sections. Figure 3.3 on the next page is a detailed sketch of one of a control volume in the domain. A typical node (i,j) in Figure 3.2 is also referred to as node P. The (i+1,j) and (i-1,j) neighbours of P are designated E for east and W for west, respectively. The (i,j+1) and (i,j-1) neighbours of P are referred to as N and S for north and south, respectively. The small letters w,e,s and n is referring to the grid lines that define the control volume faces. Figure 3.3 also defines some geometric variables. Since a non uniform grid is used, in general the width, $\Delta x^+$, of a control volume will not be equal to the distances $dx_{WP}^+$ and $dx_{PE}^+$ between P and its east and west neighbours. Regardless of the grid spacing P is always located in the geometric center of its control volume.
A non uniform block structured orthogonal grid was used in this study. Three blocks, associated with the sub domains defined by the lengths $L_F$, $L_P$ and $L_R$ respectively, can be identified by considering Figure 3.2. The blocks were designed so that the grid was made finer close to the probes leading and trailing edge in the stream wise direction and finer close to the wall in the normal direction. The reason was that high concentration gradients were expected in those regions.

![Figure 3.3: Geometric variables for a typical control volume](image)

### 3.2.2 Spatial discretization

The finite volume method was used to transform the governing equations to a system of discrete equations for the nodal values of $C^+$. Since the flow of interest is highly convective, and is dominated by high Peclet numbers the hybrid differencing scheme was used for the spatial discretization. The scheme is a combination of central and upwind differencing scheme. The central differencing scheme, which is accurate to second-order, is employed for Peclet numbers ($2Pe < 2$) and the upwind scheme, which is accurate to first order but accounts for transportiveness, is employed for large Peclet numbers ($2Pe \geq 2$). The hybrid differencing scheme is also fully conservative and unconditionally bounded.

The following result was obtained for the steady equation, $S^+y^+\frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^+^2} + \frac{\partial^2 C^+}{\partial x^+^2}$:

$$a_p C_p^+ = a_w C_w^+ + a_E C_E^+ + a_s C_s^+ + a_N C_N^+ + S_u$$

$$a_p = a_w + a_E + a_s + a_N + \tilde{A}F - S_p$$

Where $a_w$, $a_E$, $a_s$, $a_N$, are coefficients representing the influences of both convection and diffusion from neighbours $W$, $E$, $S$ and $N$ to the node $P$ respectively. The coefficients $S_u$ and $S_p$ are source terms that are only implemented for the nodal points that have boundary nodes as neighbours. The coefficients for each node are calculated, with the hybrid difference scheme, as follows:

$$a_w = \max\left[F_w, D_w + \frac{F_w}{2}\right], \quad a_E = \max\left[D_e - \frac{F_e}{2}, 0\right]$$

$$a_N = D_n, \quad a_s = D_s, \quad \tilde{A}F = F_e - F_w$$

(3.3)
Where \( F \) and \( D \) are the convection and diffusion coefficients defined as:

\[
F_w = S_y y^+ P w^+ y^+ , \quad F_e = S_y y^+ P e^+ y^+ \quad (3.5)
\]

\[
D_w = \frac{\tilde{A} y^+}{dx^+_{wp}} , \quad D_e = \frac{\tilde{A} y^+}{dx^+_{pe}} , \quad D_s = \frac{\tilde{A} x^+}{dx^+_{sp}} , \quad D_n = \frac{\tilde{A} x^+}{dx^+_{pn}} \quad (3.6)
\]

In the Matlab code, the coefficients \( a_R \) (\( R=P,W,E,S,N \)), \( F_r \) (\( r=w,e \)), \( D_b \) (\( b=w,e,s,n \)), \( S_u \) and \( S_p \) are stored in the variables \( aR(i,j) \), \( Fr(i,j) \), \( Db(i,j) \), \( Su(i,j) \) and \( Sp(i,j) \) respectively. The dimensionless concentration \( C^+_P \) and the dimensionless wall velocity gradient \( S^+ \) are stored in the variables \( C(i,j) \) and \( S \) respectively.

### 3.2.3 Implementation of the boundary conditions

The boundary conditions were incorporated into the discretised equations implicitly. For the nodes that have boundary nodes as neighbours the relevant coefficients \( a_R \) were set to zero and the inclusion from the boundaries was implemented via the terms \( S_p \) and \( S_u \).

### 3.2.4 Time discretization

The discretization above is valid for solving the steady equation. The unsteady equation,

\[
\frac{\partial C^+}{\partial t^+} + S^+_y y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^+ \partial y^+} + \frac{\partial^2 C^+}{\partial x^+ \partial x^+}
\]

was discretised in time with the Crank-Nicolson method.

The scheme is a second order implicit discretization scheme. It is unconditionally stable and has low numerical diffusion.

The consequence of using a sinusoidal time varying input signal \( S^+ \) (or of course for any type of time varying signal) as used in this study is that the convective coefficients \( F_r \) and convective boundary conditions will change in time since they depend on \( S^+ \).

### 3.2.5 Solver

The discretised equations were solved, and a concentration field \( C(i,j) \) was obtained iteratively with the TDMA method. The method is fast, computationally inexpensive and requires a minimum amount of storage. Consider the grid in Figure 3.2 again. To solve the discretised equation TDMA was applied first for the gridlines in the normal direction and then for the gridlines in the stream wise direction, also known by the south-north and west-east sweep direction respectively.

### 3.2.6 Convergence criteria

The solution was considered to be converged when the calculated total mass transfer did not change between to spatial iterations. The total mass transfer was defined in Section 1 as

\[
K^+ = L_p \int_{L_p} \frac{\partial C^+}{\partial y^+} |_{y=0} dx^+
\]

In terms of variables stored in the Matlab code the mass transfer were calculated as:

\[
\sum_{i=N_{\text{first}}}^{N_{\text{last}}} L_p * \frac{C(i,2)}{y_{\text{node}(i,2)}} * (x_{\text{grid}(i, j)} - x_{\text{grid}(i - 1, j)})
\]

Where \( N_{\text{first}} \) and \( N_{\text{last}} \) are variables stored in the Matlab code corresponding to the location of the first and last node in the i-direction within the probe domain \( L_p \).
3.3 Grid Independence studies

A grid independence study is of considerable importance when obtaining a numerical solution. Grid independence study is important to make sure that the truncated terms of Taylor series expansion, representing the derivatives, have negligible effects on the solution. As a result a grid independent discrete solution represents an accurate representation of the required solution for the continuous equations. A suitable grid to obtain grid independent result, is a grid for which more refinement does not affect the quality of the solution.

A geometry independence test is also very important to assure that the boundary conditions are physically valid so that the solution that is obtained is physical.

The grid and geometry independence study was conducted only for the discretised steady mass balance equation, \( S^+ \frac{\partial C^+}{\partial x^+} + \frac{\partial^2 C^+}{\partial y^+^2} + \frac{\partial^2 C^+}{\partial x^+^2} \). The grid and dimensions that were shown to give a grid and geometry independent solution were assumed also to be suitable for the discretised unsteady mass balance equation.

The thickness of the concentration boundary layer and the mass transfer depend on the magnitude of the input signal \( S^+ \) that is used in the simulation (i.e. depending on the input signal an independence study would give different results). The independence studies shown in this section are conducted for \( S^+ = 5000 \). It has been shown that the suitable grid for \( S^+ = 5000 \) also is suitable for input signals of low magnitude, \( S^+ = 500 \), and for high magnitude \( S^+ = 50000 \). These results are not included in this report.

3.3.1 Grid independence study

The grid independence test was conducted on four different grid sizes with the following properties.

<table>
<thead>
<tr>
<th>Grid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain L_F</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
</tbody>
</table>

Table 3.1 Grids used in the mesh independence test
For a computational domain:

![Grid and computational domain](image)

**Figure 3.4 Grid and computational domain**

With:

\[ L_F = 0.5, \ L_P = 1, \ L_R = 2, \ H = 1 \]

As seen from Figure 3.4 the grids were refined in areas where high concentration gradients were expected. It was assured for every grid that the maximum growth rate of the grid spacing, \( \frac{\Delta x_{i+1}}{\Delta x_i} \), was less than 1.05 since it otherwise, if it is higher, might cause instability problems.

When the solution had converged, the quantities that was studied and compared between the different grids were the total mass transfer \( K^+ \) and the derivative of \( C^+ \) with respect to \( y^+ \),

\[
\frac{\partial C^+}{\partial y^+}\bigg|_{y^+=0}
\]

for the nodes at the probe surface. The derivative was calculated as the concentration at the first node in the y-direction divided by the distance from the wall to the node. These values were plotted for the nodes along the probe length \( L_P \) for the four different grid sizes in Table 3.1.

**Result**

Table 3.2 shows the mass transfer, and Figure 3.5 and 3.6 show the concentration gradients for the four grids. As seen from Figure 3.6 the curves for Grid 3 and Grid 4 collapse and the difference between the mass transfer for the two solutions is 0.07 %. Hence, the solution obtained with Grid 3 is considered as grid independent.

<table>
<thead>
<tr>
<th>Grid</th>
<th>Mass transfer ( K^+ )</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>13.878</td>
<td>0.64</td>
</tr>
<tr>
<td>2</td>
<td>13.932</td>
<td>0.25</td>
</tr>
<tr>
<td>3</td>
<td>13.957</td>
<td>0.07</td>
</tr>
<tr>
<td>4</td>
<td>13.967</td>
<td>0</td>
</tr>
</tbody>
</table>

**Table 3.2** The converged values of the mass transfer and the error in percent compared to Grid 4, for the grids used in the grid independence test.
By zooming in the above figure it was seen that the differences for the grids were found at the leading and trailing edge of the probe (shown in Figure 3.6 below). For other $x^+$-values the differences were small.

As seen in Figure 3.6 the curves corresponding to Grid 3 and Grid 4 collapse well at the leading edge of the probe.
3.3.2 Geometry independence study

The geometry of the domain used in the grid independence study was made sufficiently big to make the boundary conditions physically valid. This has been achieved by increasing the size of the computational domain and study the effect of that change on the solution. Making the computational domain bigger does not change the solution.

The solution obtained by Grid 3 craved however a substantial amount of data capacity to converge. For that reason it was investigated if and how the solution changed if the computational domain was made smaller.

Consider Figure 3.7 below. The plot shows some concentration contours for the solution obtained by using Grid 3.

![Concentration contours for solution obtained by using Grid 3](image)

Figure 3.7 Concentration contours for solution obtained by using Grid 3

The figure shows that the concentration boundary layer is thin and lies in the vicinity of the wall. A domain as high as H=1 may not be necessary to get a physically valid solution. Further, with a flow from left to right, as the mass transfer occurs at $0.5 < x^* < 1.5$, there might also not be necessary with a length of the downstream probe-edge $L_R$ as high as $L_R = 2$. Hence, by reducing the size of the computational domain one might save a substantial amount of computer capacity and still have physical valid boundary conditions.

The domain was changed so that:

$L_F=0.5$, $L_P=1$, $L_R=0.5$ (changed), $H=0.5$ (changed)

And the amount of cells in Domain $L_R$ and the normal direction were changed according to table 3.3 below.

<table>
<thead>
<tr>
<th>Grid</th>
<th>Domain $L_F$</th>
<th>Domain $L_P$</th>
<th>Domain $L_R$</th>
<th>Normal direction</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>80</td>
<td>160</td>
<td>80</td>
<td>80</td>
<td>320 x 80</td>
</tr>
</tbody>
</table>

Table 3.3 Grid used in the geometry independence test
Result
Table 3.4 shows the mass transfer and Figure 3.8 show the concentration gradients for three grids. As seen from Figure 3.8 the curves corresponding to the grid for the changed domain, Grid 3, and the grid that was shown to give a grid independent solution in the previous section, Grid 5, collapse perfectly. As seen from table 3.4, the difference in mass transfer between the two solutions is negligible (0.7%-0.8% deviation from the finest grid, Grid 4). I.e. by changing the geometry the solution has not changed. Hence, the solution obtained with Grid 5 is considered to be grid and geometry independent and is the grid that is used in the report.

<table>
<thead>
<tr>
<th>Grid</th>
<th>Mass transfer K⁺</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>13.967</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>13.956</td>
<td>0.08</td>
</tr>
</tbody>
</table>

Table 3.4 The converged value of the mass transfer and the error in percent compared to Grid 4, for the grid used in the geometry independence test.

Figure 3.8 \( \frac{\partial C^+}{\partial y^+} \) for the nodes at leading edge of the probe

Figure 3.9 The grid used in the report, Grid 5
Discussion
A grid that gave a grid and geometry independent solution was obtained. As mentioned in the beginning of this section the independence studies were only made for the steady state simulation. A comparison of the values of mass transfer for the simulation of the unsteady mass balance equation after reaching steady state with the simulation of the steady mass balance equation for $S^+=500$ $S^+=5000$ and $S^+=50000$ respectively was made. The solutions matched each other with at least a ten-digit accuracy, as seen below. This gives some confidence regarding the adequacy of using the same grid in the unsteady simulation.

\[
S^+=500
\]

Steady mass balance equation: $K^+=6.63530660249650$
Unsteady mass balance equation: $K^+=6.63530660249758$

\[
S^+=5000
\]

Steady mass balance equation: $K^+=13.9583723411284$
Unsteady mass balance equation: $K^+=13.9583723411721$

\[
S^+=50000
\]

Steady mass balance equation: $K^+=29.8143687611145$
Unsteady mass balance equation: $K^+=29.8143687612464$

3.3.3 Time step independence study
For an unsteady problem it is, except from doing a grid independence study, also of major importance to do a time step independence study. A time step for which a time step independent result is achieved, is sufficiently small so that if it is decreased, it doesn’t affect the quality of the solution.

Let the dimensionless parameter c, the Courant number be defined.

\[
c = \frac{U^+ \Delta t^+}{\Delta x^+} \tag{3.7}
\]

This quantity is the ratio of time step $\Delta t^+$ to the characteristic convection time, $\Delta x^+/U^+$, the time required for a fluid particle to be convected a distance $\Delta x^+$. For high convective flows the criteria that needs to be satisfied is

\[
c < 1 \text{ or } \Delta t^+ < \frac{\Delta x^+}{U^+} = \frac{\Delta x^+}{S^+ y^+} \tag{3.8}
\]

Criteria (3.8) indicates that the critical cells are the ones associated with small $\Delta x^+$ and a high velocity $U^+$. If the criteria is fulfilled for those cells it is automatically fulfilled for the other cells. The critical cells in the particular problem are the small cells at the top of the domain with $x^+$-values corresponding to the probes leading and trailing edge. Because of the linear velocity profile, $U^+=S^+ y^+$, the highest speed of the fluid particles will be found at the highest located cells in the domain. And since the grid is refined at the leading- and trailing edge the cells with the smallest $\Delta x^+$ will also be found here.
The input signals $S(t^+)$ that will be used in studying the frequency response of the probe in this study are the following:

Low $S^+$: \[ S^+_{LS^+} = 500 + 10 \sin(2 \delta f^+ t^+) \]

Medium $S^+$: \[ S^+_{MS^+} = 5000 + 100 \sin(2 \delta f^+ t^+) \]

High $S^+$: \[ S^+_{HS^+} = 50000 + 100 \sin(2 \delta f^+ t^+) \]

Now it will be showed that solutions for conditions of $S^+_{MS^+}$ is time step independent. If criteria (3.8) is fulfilled for the maximum value of $S^+_{MS^+}$, which via the linear relation $U^+ = S^+ y^+$ is connected to the maximum value of velocity, then it is fulfilled for any lower value of $S^+_{MS^+}$.

Geometrical data for the critical cell at the top of the domain read: 
\[ \Delta x^+ = 0.0028, \ y^+ = 0.4948 \]
and with:
\[ S^+_{MS^+} = 5100, \text{ criteria (3.8) gives: } \Delta t^+ < \frac{0.0028}{5100 \times 0.4948} = 1.11 \times 10^{-6} \]

The time step was chosen to a lower value $\Delta t^+ = 1 \times 10^{-6}$ \hfill (3.9)

The Matlab code for the unsteady mass balance equation was run with the initial condition $C^+ = 1$ for all the nodes in the domain. Two solutions corresponding to the two time steps,
\[ \Delta t^+ = 1 \times 10^{-6} \hfill (3.9) \]
\[ \Delta t^+ = \frac{1 \times 10^{-6}}{2} = 5 \times 10^{-7} \hfill (3.10) \]
were obtained and compared at the same time $t^+ = 5 \times 10^{-4}$.

**Result**

Consider the concentration matrix $C$, containing the concentration $C^+$ for every nodal point, corresponding to each solution. By subtracting the concentration matrixes it was found that the maximum absolute error in a node was $2.24 \times 10^{-7}$. This indicates that the solutions were almost identical.

To visualize this, let for example the concentration at the second y-node as a function of $x^+$, for the two different solutions be plotted.
Figures 3.10 and 3.11 show that the concentrations profiles for $t^+ = 5 \times 10^{-4}$ are identical for the two different time steps (with an error about $1 \times 10^{-7}$). The solution does not change by using (3.10), i.e. reducing the time step to half of the value given by criteria (3.8). Hence, the solution obtained by using (3.9), $\Delta t^+ = 1 \times 10^{-6}$ is time step independent.

The same study was conducted for the cases for the low and high $S^+$ input signals and it was found that the solution was time step independent for $\Delta t^+ = 1 \times 10^{-6}$ and $\Delta t^+ = 1 \times 10^{-7}$ respectively.

3.3.4 Validation of the codes

Comparisons with analytical solutions have been made to validate the codes. The results from those tests show that the way of implementing the time and spatial discretization schemes and solving the resulting set of algebraic equations with the TDMA solver is correct for a non-uniform grid. Those studies are shown in Appendix 1-2.
Section 4: Numerical Simulations

4.1 Steady mass balance equation

In this section the results of the numerical simulation of the steady state mass balance equation are gathered and interpreted. Two equations has been solved, one that takes the x-diffusion into account Eq. (4.1) and one that does not Eq. (4.2).

**Case 1:**

\[
S^+ y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^+^2} + \frac{\partial^2 C^+}{\partial x^+^2} \quad (4.1)
\]

**Case 2:**

\[
S^+ y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^+^2} \quad (4.2)
\]

Having defined boundary conditions, and by introducing a constant input signal, a velocity gradient \( S^+ \), the discretised forms of Eqs. (4.1) and (4.2) have been solved numerically, i.e. the concentration \( C^+ \) in every nodal point has been calculated. Consequently, by knowing the concentration field, the mass transfer \( K^+ \) can be calculated. Numerical simulations for a large range of constant input signals, \( 250 \leq S^+ \leq 60000 \), are to be conducted and the corresponding mass transfers will be calculated. The relation between \( S^+ \) and \( K^+ \) for that range of \( S^+ \) will be represented in a figure.

Eq. (4.2) can also be solved analytically. Mitchell and Hanratty (1966) showed that for the analytically calculated concentration distribution the mass transfer \( K^+ \) is related to \( S^+ \) as:

\[
K^+ = 0.807S^{4/3} \quad (4.3)
\]

Neglecting the x-diffusion has been shown to be valid for \( S^+ \geq 5000 \) (Ling, 1962)

The following discussion includes a comparison between the numerically calculated values of \( K^+ \) for Case 1 when x-diffusion is taken into account, for Case 2 where it is not and with the values of \( K^+ \) given by the analytical expression (4.3).
4.1.1 Results
Figure 4.1 shows the concentration contours for a steady flow over a probe, obtained with the numerical solution of Case 1 with $S^+ = 5000$. As the flow from left to right approaches the probe the fluid particles start to lose concentration to the probe and a concentration boundary layer is developed. The uppermost curve represents the contour for which the concentration values are 99 percent of the bulk concentration, $C^+ = 0.99$, i.e., the definition of the boundary layer thickness. It is also notable that the concentration boundary layer starts developing even before the leading edge of the probe. This is however natural since the x-diffusion allows the fluid particles, before passing the leading edge, to feel the presence of the probe.

![Concentration contours for Case 1 $S^+ = 5000$](image1)

Figure 4.1 Concentration contours for Case 1 $S^+ = 5000$

Figure 4.2 below shows how the concentration profiles develop over the probe surface $0.5 < x^+ < 1.5$. The concentration $C^+$ as a function of $y^+$ for some $x^+$-values along the probe is plotted. A deeper look in the figure shows that the curves are steepest at the leading edge at the probe and reaches the bulk concentration at low $y^+$-values. As moving towards the trailing edge the steepness of the curves decreases and reach the bulk concentration at higher $y^+$-values.

A physical interpretation can be made by considering a fluid particle moving from left to right over the probe surface. The particle approaching the leading edge has initially high concentration. As moving from left to right over the probe surface it continuously looses concentration. Hence, the difference in concentration between the probe surface ($C^+=0$) and the particle above becomes smaller and smaller, and the thickness of the concentration boundary layer increases.

![Concentration profiles for Case 1 $S^+ = 5000$](image2)

Figure 4.2 Concentration profiles for Case 1 $S^+ = 5000$
**Influence of different values of $S^+$**

It was investigated how the numerical solution of the steady problem changed when changing $S^+ = \frac{S L_p^2}{D}$. For a given diffusion constant $D$ and probe length $L_p$, increasing $S^+$ is the same as increasing the velocity gradient $S$, i.e. increasing the convection.

**Case 1**

Figure 4.3 and Table 4.1 below show the boundary layers development and total mass transfer for three different values of $S^+$. Figure 4.3 reveals that when increasing the velocity gradient the boundary layer becomes thinner. Further it shows that the boundary layer starts to develop closer to the leading edge as the $S^+$ gets higher. This is a result of a weaker influence of the $x$-diffusion.

Table 4.1 shows that the total mass transfer increases when increasing $S^+$.

![Figure 4.3](image)

**Figure 4.3** Boundary layer thickness and development for different values of $S^+$ for Case 1. The contour shown corresponds to $C^+=0.99$

<table>
<thead>
<tr>
<th>$S^+$</th>
<th>$K^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>6.635</td>
</tr>
<tr>
<td>5000</td>
<td>13.955</td>
</tr>
<tr>
<td>50000</td>
<td>29.814</td>
</tr>
</tbody>
</table>

**Table 4.1** Values of $K^+$ for three values of $S^+$ for Case 1

The thinner boundary layer and the greater mass transfer can be physically interpreted due to the increased rate of convection. Since the speed of the particles increases, more particles with high concentration will approach the leading edge of the probe and pass the probe surface faster for a given period of time. This contributes to maintain a higher concentration gradient and thus a thinner boundary layer and a higher mass transfer.
Case 2
As seen from Figure 4.4 and Table 4.2 below, the boundary layers and the mass transfers look a bit different for Case 2. Considering that the flow is from left to right, the absence of the x-diffusion term hinders a transport of information opposite the flow direction, i.e. from right to left. The effect of neglecting the x-diffusion term is therefore seen as a boundary layer development first at the leading edge. Neglecting the x-diffusion gives also a lower value of mass transfer $K^+$ than for Case 1.

![Figure 4.4](image)

*Figure 4.4* Boundary layer thickness and development for different values of $S^+$ for Case 2. The contour shown corresponds to $C+=0.99$

<table>
<thead>
<tr>
<th>$S^+$</th>
<th>$K^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>6.404</td>
</tr>
<tr>
<td>5000</td>
<td>13.797</td>
</tr>
<tr>
<td>50000</td>
<td>29.726</td>
</tr>
</tbody>
</table>

*Table 4.2* Values of $K^+$ for three values of $S^+$ for Case 2
Comparing with analytical solution
To investigate further how $K^+$ depended on the magnitude of $S^+$ numerical simulations were made for values of $S^+$ in a considerable large range: $250 \leq S^+ \leq 60000$.
Simulations were conducted for both Case 1 and Case 2 in order to see the effect on $K^+$ when neglecting x-diffusion. As mentioned in the introduction, if the x-diffusion term in the steady mass balance equation is neglected the equation has an analytic solution and the mass transfer is calculated as:

$$K^+ = 0.807S^{+1/3}$$  \hspace{1cm} (4.3)

The calculated values of $K^+$ for the two cases will be compared to expression (4.3)

Case 2
Figure 4.5 shows the calculated values of $K^+$ for a substantial amount of input signals $S^+$ when the x-diffusion is neglected. In the same figure the values obtain with the analytic expression (4.3) is plotted. Consider Figures 4.5 and 4.6 below. It can be seen that the values of $K^+$ achieved with numerical simulation of Case 2 are almost identical with the values given by expression (4.3), with a maximum difference about 0.017 %. This is a further verification that the Matlab code is written correctly.

Case 1
Numerical simulations for Case 1 were conducted and the calculated values of $K^+$ were compared with Eq. (4.3). Such a study would reveal what kind of effect the x-diffusion term had on the values of $K^+$. When increasing $S^+$ the ratio between the convection and diffusion increases and the diffusion becomes less important. Hence, a hypothesis would be that
numerical solution for a high value of $S^+$ would give a mass transfer which would not differ much from the value given by the analytical expression (4.3). The simulations were made in same range of $S^+$ as for Case 2 above: $250 \leq S^+ \leq 60000$

Figure 4.7 and 4.8 show that there is a good agreement between the values of mass transfer calculated numerically and analytically for the whole range of $S^+$, and in particular for high values of $S^+$. Figure 4.7 reveals that the values corresponding to the numerical simulation are somewhat higher than the values calculated with the analytical expression (the difference was better seen in a log-log scale). Judging by Figure 4.8, the difference between the values from the analytical expression and the numerical simulation decreases when increasing $S^+$. This confirms the hypothesis stated above, that suggested that the difference should be smaller when the x-diffusion played a less important role. For values of $S^+ > 5000$ the difference is less than 1.2 %. However, for lower values than $S^+ < 500$ the x-diffusion should be taken in consideration.

An analysis of how the x-diffusion contributes to a higher mass transfer has also been made. This study is attached in Appendix 3. The analysis concludes that the x-diffusion term plays an important role at the probes leading and trailing edge and contributes to a locally higher mass transfer in those regions. This effect was however shown only to have some importance for low values of $S^+$ and becomes less important as $S^+$ gets higher.
Experimental use
A relation between the mass transfer $K^+$ and the velocity gradient $S^+$ has been obtained by numerical simulation and is presented in Figure 4.7. Consider a mass transfer probe that is mounted in a steady flow to measure the mass transfer experimentally. The relation between $K^+$ and $S^+$ that has been obtained makes it possible to translate a measured mass transfer into a velocity gradient. If the viscosity of the fluid is known, the wall shear stress can consequently be calculated.

Conclusion
A Matlab code that solves the steady mass balance equation has been developed. Numerical simulations for a large range of constant input signals, $250 \leq S^+ \leq 60000$, have been conducted and the corresponding mass transfers have been calculated. The relation is represented in a figure, and can be used to translate an experimental measured mass transfer to a velocity gradient and a wall shear stress. A study of how the solutions change when neglecting the x-diffusion term has been conducted. The differences are noted as slightly different appearances of the concentration boundary layers and values of mass transfer $K^+$. When the x-diffusion is neglected the numerically and analytically calculated values of $K^+$ are almost identical which indicates that the Matlab code is written correctly. If the x-diffusion is taken into consideration the simulations give a somewhat higher value of $K^+$. The difference is however small and for $S^+ \leq 5000$ less than 1.2 \%.
This study therefore also verifies the validity of using the analytic expression, $K^+ = 0.807S^{+1/3}$ for calculating the mass transfer for $S^+ \leq 5000$. 
4.2 Unsteady mass balance equation

The former chapter focused on the steady mass balance equation. In this chapter, the results from numerical simulations of the unsteady mass balance equation (4.4) will be presented and analyzed.

\[
\frac{\partial C^+}{\partial t^+} + S^+ \frac{\partial C^+}{\partial y^+} = \frac{\partial^2 C^+}{\partial y^+^2} + \frac{\partial^2 C^+}{\partial x^+^2} \tag{4.4}
\]

The discretized form of equation (4.4) was solved numerically by introducing a time and frequency depending sinusoidal input signal \( S^+(t^+, f^+) \) as depicted in Figure 4.9 below.

![Sinusoidal input signal](image)

**Figure 4.9 Sinusoidal input signal**

Instead of a constant input signal the input signal \( S^+ \) was defined as the sum of time average property \( \overline{S^+} \) and fluctuating property \( s^+ \) in a similar way as the Reynolds decomposition:

\[
S^+ = \overline{S^+} + s^+ \tag{4.5}
\]

Now, defining the fluctuating property as a sinusoidal function, (4.5) reads:

\[
S^+ = \overline{S^+} + \hat{s}^+ \sin(2\pi f^+ t^+) \tag{4.6}
\]

Where in \( \hat{s}^+ \) and \( f^+ \) are the amplitude and the frequency of fluctuating property \( s^+ \) respectively.

**Frequency response**

Since the input signal \( S^+ \) varies with time, the output signal \( K^+ \) will consequently also vary with time. Most of the work on the frequency response of mass transfer probes has involved an assumption that the amplitude of the fluctuations is small compared to the time-average flow. It has been shown by Mitchell Hanratty (1966) that when introducing an input signal with low amplitude fluctuations, \( \hat{s}^+ \ll \overline{S^+} \), the calculated output signal is also a sinusoidal function. It fluctuates with the same frequency as the input signal, but is phase delayed with an angle \( \Delta \Theta \) and damped.

\[
K^+ = \overline{K^+} + \hat{k}^+ \sin(2\pi f^+ t^+ + \Delta \Theta) \tag{4.7}
\]
It has been shown that the magnitude of the damping and phase delay is strongly depending on the magnitude of the input frequency. This frequency depending behavior of $K^+$ is called the frequency response of the mass transfer probe.

The objective was to investigate, via numerical simulation of the discretised unsteady mass balance equation, the frequency response of the mass transfer probe. Simulations for both taking into account and neglecting the x-diffusion term \( \frac{\partial^2 C^+}{\partial x^+^2} \) were conducted.

The results are analyzed and compared with the frequency response taken from Py (1990). That frequency response was obtained by solving the mass balance equation neglecting the x-diffusion and is valid for low amplitude fluctuations, \( \frac{\hat{\delta}^+}{\delta S^+} \leq 0.05 \) for any \( S^+ > 5000 \).

The input signals used in this study were the following:

- Low $S^+$: \( S^+_{LS^+} = 500 + 10\sin(2\,\delta f^+ t^+) \)
- Medium $S^+$: \( S^+_{MS^+} = 5000 + 100\sin(2\,\delta f^+ t^+) \)
- High $S^+$: \( S^+_{HS^+} = 50000 + 1000\sin(2\,\delta f^+ t^+) \)

With the ratio on \( \frac{\hat{\delta}^+}{\delta S^+} = \frac{10}{500} = \frac{100}{5000} = \frac{1000}{50000} = 0.02 \) for one and all the three different input signals. The reason was to maintain a ratio of \( \frac{\hat{\delta}^+}{\delta S^+} \leq 0.05 \) to make a comparison to the frequency response reported by Py (1990). The reason for doing simulation for three different input signals was to investigate if the frequency response depended on the magnitude of $S^+$. 

\[
\text{Damping} = 3 \frac{k^+}{K^+} \frac{\hat{\delta}^+}{S^+} \quad (4.8)
\]
4.2.1 Results
Previous studies have shown that when increasing the frequency of the input signal the output signal gets damped and a phase delay occurs (Mitchell Hanratty (1966), Fortuna, Hanratty (1971) and Py (1990)).
This may be interpreted physically as it takes a while for the system to feel a change of the input signal, because of the natural inertia inherent to the system. When the frequency gets higher the system have less time to reach the steady state values of $K^+$ and further it exhibits peaks after the peaks of $S^+$. The response is damped and delayed.

Figures 4.10 to 4.12 show some results obtained by the numerical simulation for the low $S^+$ input signal. Studies of the output signal $K^+$ verifies that it oscillates with the same frequency as $S^+$. The figures show clearly that when the frequency increases, there is a strong unsteady effect; The amplitude of the output signal $K^+$ decreases and the phase delay increases with an increasing frequency.

![Figure 4.10 Response $f_{\text{prim}}=0.2$](image)

![Figure 4.11 Response $f_{\text{prim}}=1$](image)

![Figure 4.12 Response $f_{\text{prim}}=5$](image)

In the previous studies the non dimensionalisation was made in a slightly different manner than this study. To compare the frequency response for the same frequencies the
dimensionless frequency \( f^* \) was scaled to \( f^ \text{prim} = f^* S^* \). In order to see the behaviour of both the input signal and the output signal \( S^* \) was scaled down to \( S^ \text{prim} = \frac{0.807}{S^*^{2/3}} \).

The whole frequency range
Numerical simulation for the three different input signals,
- Low \( S^+ \): \( S_{LS}^+ = 500 + 10\sin(2 \delta f^* t^*) \)
- Medium \( S^+ \): \( S_{MS}^+ = 5000 + 100\sin(2 \delta f^* t^*) \)
- High \( S^+ \): \( S_{HS}^+ = 50000 + 1000\sin(2 \delta f^* t^*) \)
was made for some certain values of frequency within the range \( 0 \leq f^ \text{prim} \leq 10 \). The phase delay and damping was then calculated.

The damping was calculated with a function defined as,
\[
\text{Damping} = 3 \frac{\dot{K}^*}{K^*} \frac{\dot{S}^*}{S^*} \tag{4.8}
\]
and is a measure of how much \( K^* \) deviates from the steady state solution. And the phase delay as,
\[
\Delta \Theta = 2 \pi f^* \Delta t^*_{sk} \tag{4.9}
\]
where \( \Delta t^*_{sk} \) is the time between the peak of the input signal \( S^* \) and output signal \( K^* \) as depicted in Figure 4.13 below.

![Figure 4.13 Input and output signal](image)

Figures 4.14 to 4.17 on the following pages show a compilation of frequency response obtained with the numerical simulation. The frequency response predicted by Py (1990) is plotted for comparison.
**Frequency response**
The result from the numerical simulations in this study verifies that the system has a damping and phase delaying effect on $K^*$ that depends on the frequency of the input signal. The result shows that when neglecting the x-diffusion the frequency response is different.

For numerical simulations when the x-diffusion is neglected the results show an identical frequency response for the three different input signals. When the x-diffusion is taken into account the results show a different appearance of the frequency response for each three of the different input signals.
The frequency response agrees fairly well with previous results by Py (1990).

**Damping**
Figure 4.14 reveals the increasing damping of the output signal as the frequency increases. The figure further shows that the result from the numerical simulation follows the same trend as the solution obtained by Py (1990).

With x-diffusion
It is observed that the damping of the output signal, for a given frequency, is different for the three input signals. The output signals are less damped as $S^+$ is increased.

Without x-diffusion
When the x-diffusion is neglected the figures show that the damping on the contrary is the same for the three different input signals. The signals are also less damped in comparison with the signals where x-diffusion was taken into account.

![Figure 4.14: Damping as a function of frequency](image-url)
Another interesting detail can be observed by studying Figures 4.15 and 4.16 below where the damping is plotted in a log-log scale. In Figure 4.16 a closer view for the high frequency domain is shown. The straight lines that have been drawn show an asymptotic behaviour of the solutions for $f_{\text{prim}}^* \geq 6$. This indicates that the damping for higher frequencies than $f_{\text{prim}}^* = 10$ can be obtained be following the corresponding asymptotic curves.

**Figure 4.15** Damping as function of frequency plotted in log log scale

**Figure 4.16** Asymptotic behaviour of the damping for high frequencies
Phase delay
Figure 4.17 below shows the increasing phase delay expressed in radians when increasing the frequency. The numerical solutions follow the same trend as the solution of Py (1990), but are lower for the whole frequency range.

With x-diffusion
Like the damping, the phase delay is different for the three input signals when x-diffusion is taken into account. The phase delay, for a given frequency is decreasing when increasing $S^*$. 

Without x-diffusion
The values of the phase delay for the three different input signals when x-diffusion is neglected are almost identical, with a maximum difference of 0.01. The signals are less phase-delayed than the signals where x-diffusion was taken into account. The difference is considerable large, especially for high frequencies. One remarkable feature is that the values show the biggest deviation from the curve taken from Py (1990). This is strange since both were calculated neglecting the x-diffusion and therefore ought to be similar.

Experimental use
The frequency response obtained in this study can be used to translate an experimentally measured time varying mass transfer to a velocity gradient. If the viscosity of the fluid is known the wall shear stress can consequently be calculated.

Discussion
The frequency response taken Py (1990) has been achieved with a different approach than the method used in this study, and some other further assumptions have been made. The unsteady mass balance equation has been broken down into two coupled equations (the time averaged equation and the equation for the fluctuating property) after doing Reynolds decomposition. The x-diffusion term and the quadratic term has been neglected and the frequency response has been calculated after solving the two coupled equations numerically (read more about this in Appendix 4).

The lack of detailed data from those studies, for example information about discretization schemes, grid- and time step-independence studies, has made it difficult to estimate the accuracy of the frequency response.
Conclusion

A Matlab code that solves the unsteady flow over a rectangular probe has been developed. Numerical simulations of the unsteady mass balance have been conducted by introducing a low amplitude sinusoidal varying input signal. The simulations have been run for three different input signals and for different frequencies. The effect of the x-diffusion has been studied by doing the simulations with and without the x-diffusion term. In this way the damping and phase delay, i.e. the frequency response, of the mass transfer probe for has been obtained for the three different input signals with and without x-diffusion term respectively.

The results show that the frequency response is not the same when neglecting the x-diffusion. On the other hand, when taking the x-diffusion into account the frequency response depends not only on the frequency but also on the magnitude of $S^+$ of the input signal. The biggest difference is noted for the phase delay.

In Section 4.1, when doing numerical simulations of the steady mass balance equation, the effect from x-diffusion on the mass transfer was shown to be negligible for $S^+ > 5000$. For unsteady simulation the x-diffusion seems to have a damping and especially phase delaying effect on the mass transfer and should not be neglected, not even for input signals higher than $S^+ > 5000$. The frequency response agrees fairly well with the one taken Py (1990). However is the difference quite substantial when it comes to phase delay. The phase delay from simulations without the x-diffusion term displays the biggest deviation from the values taken from Py (1990). Since the x-diffusion term has been neglected for both of the solution they ought to be the most similar.

In this study it has been concluded that when taking the x-diffusion into account the frequency response looks different. The x-diffusion term has demonstrably an effect on the instantaneous mass balance. In order to visualize the importance of the x-diffusion term an analysis of the balance of the terms in the fluctuating equation was chosen to be conducted. Such an analysis would also show the importance of the quadratic terms that was neglected in the study of Py (1990).

Analysing the balance

Equation (4.10) is the governing equation for the dimensionless fluctuating concentration. Since the equation is space and time dependent an extensive study of the balance of the terms in equation (4.10) in the computational domain for the three types of input signals (and different frequencies) would be computationally expensive and very time craving. As a result, the balances have been chosen to be made at two wall-normal locations within the concentration boundary for several stream wise locations. Those balances have been checked at different times but only results for a single time will be presented. Balances have been made for the three different input signals and for different frequencies but only the results from the Medium $S^+$ input signal for one frequency will be presented.

\[
\frac{\partial c^+}{\partial t} + S^+ y^+ \frac{\partial c^+}{\partial x^+} + s^+ y^+ \frac{\partial \bar{c}^+}{\partial x^+} + s^+ y^+ \frac{\partial c^+}{\partial x^+} - y^+ \frac{\partial \bar{s}^+ c^+}{\partial x^+} = \frac{\partial^2 c^+}{\partial x^+^2} + \frac{\partial^2 c^+}{\partial y^+^2} \quad (4.10)
\]

The balance was chosen to be evaluated for every $x^+$-value $0 \leq x^+ \leq 2$ for a constant $y^+$-position that lies within in the concentration boundary layer. A balance for two $y^+$-positions were made. One close to the wall, the second y-node, and one a bit further from the wall, the fifteenth y-node.
The concentration at the nodes varies in time sinusoidally. The figure below shows how an output signal $K^+$ varies over a period $T^+ = \frac{1}{f^+}$. The balances presented in this section were made for the time for which the mass transfer has its maximum value (to most left or most right value in Figure 4.18).

![Figure 4.18 The variation of $K^+$ for a period $T^+$](image)

When plotting the balances the terms in Eq. (4.10) were a bit reorganized:

$$\frac{\partial c^+}{\partial t^+} = -S^+ y^+ \frac{\partial c^+}{\partial x^+} - s^+ y^+ \frac{\partial c^+}{\partial x^+} - s^+ y^+ \frac{\partial c^+}{\partial x^+} + y^+ \frac{\partial s^+ c^+}{\partial x^+} + \frac{\partial^2 c^+}{\partial x^2} + \frac{\partial^2 c^+}{\partial y^2}$$

(4.11)

In this way all positive terms of the right hand side acts to increase the value of the fluctuating concentration $c^+$.

**Results**

The result shows that the quadratic terms (underlined in Eq. 4.11) are fully negligible in the balances made for the medium $S^+$ input signal. The result shows, as expected, that the fluctuating x-diffusion $\frac{\partial^2 c^+}{\partial x^2}$ plays an important role in the balances. Results from analysing balances for the two other input signals show the same behaviour but are not included in this report.
Second y-node

Seen from Figure 4.19 and 4.20 the x-diffusion plays a major rule at the leading and trailing edge of the probe. The convection terms were of low order and have not been included in the Figures 4.19 and 4.20. The fluctuating concentration $c^*$ has been scaled in Figs. 4.19 and 4.20 in order to be seen.

![Figure 4.19 Balance leading edge second y-node, $S_{MS^*}, f^*_{prim}=1$](image)

![Figure 4.20 Balance trailing edge second y-node, $S_{MS^*}, f^*_{prim}=1$](image)

Fifteenth y-node

The balance of the fifteenth y-node in Figure 4.21 below reveals that the x-diffusion plays a significant role in the whole domain.

![Figure 4.21 Balance 15th y-node, $S_{MS^*}, f^*_{prim}=1$](image)
Conclusion
The result indicates that the quadratic terms are fully negligible within the concentration boundary layer for the kind of low amplitude input signals used in this report. The study shows however that diffusion of the fluctuating concentration $c^+$ in the stream wise direction, \[ \frac{\partial^2 c^+}{\partial x^+^2} \], plays an important role in the balances, even for the high $S^+$ input signal. Naturally, this affects the instantaneous concentration and mass transfer and consequently the frequency response.
Section 5: Final Conclusions

The finite volume method was used to transform the partial differential mass balance equation to algebraic relations. The equation has been discretised spatially with the hybrid scheme and in time with the Crank Nicolson scheme and have been solved iteratively with the TDMA solver. In that way the concentration distribution has been obtained numerically and the mass transfer to the probe have been calculated. The codes that solve the problems have been programmed in Matlab. Comparisons with analytical solutions have been made to validate the codes. The results from those tests show that the way of implementing the time and spatial discretization schemes and solving the resulting set of algebraic equations with the TDMA solver is correct for a non uniform grid. By conducting grid independence studies it has been shown that the grid size, size of the computational domain and time steps used in the numerical simulations are appropriate. Refining the grid, making the computational domain bigger or reducing the time step do not affect the quality of the solution.

Numerical simulations of both the discretised steady and unsteady mass balance equation have been conducted. The results have been analyzed and compared with results from previous studies. In previous studies it has been concluded that the x-diffusion term in the mass balance equation can be neglected for values of the velocity gradients higher than $S^* = 5000$.

A Matlab code that solves the steady mass balance equation was developed successfully. When neglecting the x-diffusion term the mass balance equation has an analytical solution and there is an analytical relation between $S^*$ and $K^*$. Numerical simulations for a big range of $S^*$, when neglecting the x-diffusion, were conducted. The mass transfer $K^*$ for each input signal $S^*$ was calculated and a very good agreement to the analytical expression was shown, which validates the correctness of the code.

Numerical simulations for the same range of $S^*$ were conducted when taking the x-diffusion into account. The results show a slightly different appearance of the concentration boundary layers and somewhat higher values of mass transfer $K^*$. The analysis shows that the x-diffusion term contributes to a locally higher mass transfer at the probes leading and trailing edge which explains the higher values of mass transfer $K^*$. The difference is however small and for $S^* = 5000$ less than 1.2%; the effect on mass transfer when neglecting the x-diffusion is negligible for $S^*$ of that order. The relation between $K^*$ and $S^*$ that has been obtained can be used to translate an experimentally measured steady mass transfer to a velocity gradient. If the viscosity of the fluid is known the wall shear stress can consequently be calculated.

A Matlab code that solves the unsteady flow over a rectangular probe has been developed. Numerical simulations of the unsteady mass balance have been conducted by introducing a low amplitude sinusoidal varying input signal. The simulations have been run for three different input signals and for different frequencies. The effect of the x-diffusion has been studied by doing the simulations with and without the x-diffusion term. In this way the damping and phase delay, i.e. the frequency response, of the mass transfer probe for has been obtained for the three different input signals with and without x-diffusion term respectively. The frequency response can be used to translate an experimentally measured time varying mass transfer to a velocity gradient. If the viscosity of the fluid is known the wall shear stress can consequently be calculated.

The results show that the frequency response is not the same when neglecting the x-diffusion.
For unsteady simulation the x-diffusion seems to have a damping and especially phase delaying effect on the mass transfer and should not be neglected, not even for input signals higher than $S^r > 5000$. The frequency response agrees fairly well with the one taken by Py (1990). However, the difference is quite substantial when it comes to phase delay. The differences are probably due to that Py has solved the equation in a different manner than the one conducted in this study.
Bibliography


Appendix

Appendix 1 - Comparing with a steady state analytical solution

To see if the way of implementing the hybrid discretization scheme for the steady mass balance equation and the TDMA solver were correct, a comparison between an analytical solution was going to be made.

Analytical solution

A concentration $C^+$ is transported by means of convection and diffusion through the one-dimensional domain sketched in Figure A1.1.

\[
\begin{align*}
C_0^+ & \quad \text{\textup{u}^+} \quad C_L^+ \\
0 & \quad i = 0 \quad L & \quad i = L
\end{align*}
\]

Figure A1.1 1-D convection diffusion

An analytical solution for such a problem is known and reads:

\[
C^+(i^+) = C^+_0 + C^+_L - C^+_0 \frac{\exp(u^+ i^+) - 1}{\exp(u^+ L) - 1} \quad \text{(A1.1)}
\]

With boundary conditions defined as

\[
C^+_0 = 1 \quad \text{and} \quad C^+_L = 0 \quad \text{(A1.2)}
\]

(A1.1) becomes:

\[
C^+(i^+) = 1 - \frac{\exp(u^+ i^+) - 1}{\exp(u^+ L) - 1} \quad \text{(A1.3)}
\]

1-D convection and diffusion in x-direction

Eq. (A1.3) was implemented in the matlab code to examine the analytical concentration distribution in the x-direction ($i=x$), i.e. the concentration at the position of every x-node in a one dimensional domain with length $L=1$ and a constant velocity $u^+ = 10$. For a uniform grid with 25 cells in the x-direction the following the result was obtained.
Numerical Solution
The result was then going to be compared with a numerical solution obtained by using the hybrid discretization scheme with TDMA solver.

1-D convection and diffusion in x-direction
By modifying the domain, letting the constants $a_S$ and $a_N$ equal zero, and implying the corresponding boundary conditions (A1.2) the code was modified to fit for the problem stated in Figure A1.1.
As seen from Figure A1.2 the concentration gradient is high for high x-values. Solution for two types of grids were obtained: For a uniform grid with 25 cells and a for non uniform grid with 25 cells for which the grid was refined for high x-values.

Results
The solution obtained by the numerical method is accurate, and remarkably good.
As seen from Figure A1.3, the curves corresponding to the analytical and numerical solution collapse (for graphic reason the solution obtained with the uniform grid is not plotted in the same figure). Judging by Figure A1.4 the error between the analytical solution and the numerical one was made even smaller by refining the grid were high concentration gradients were found. The biggest percentage error for the non uniform grid for every node is smaller than 0.25.

1-D convection and diffusion in y-direction
A similar study was performed for convection diffusion in the y-direction with the same results.

Conclusion
The results indicates that the way of implementing the hybrid differencing scheme, and solving it with a TDMA solver is correct for both a uniform and non uniform grid for 1-dimensional convection diffusion problem.
Appendix 2 - Comparing with an unsteady state analytical solution

To see if the way of implementing the Crank Nicolson method for discretizing the unsteady equation and the TDMA solver were correct, a comparison with an analytical solution was performed.

Analytical solution

The analytical solution for diffusion in a semi infinite fluid reads:

\[
\frac{\partial C^+}{\partial t^+} = \frac{\partial^2 C^+}{\partial i^{+2}}
\]

(A2.1)

\[
C^+ = C^+(i^+, t^+)
\]

Figure A2.1 Semi infinite fluid

A solution to eq. (A2.1) is known for the case with constant surface concentration \( C^+(0, t^+) = C_s^+ \) and an initial condition \( C^+(i^+, 0) = C_0^+ \) and reads:

\[
C^+(i^+, t^+) = \left( C_0^+ - C_s^+ \right) \text{erf} \left( \frac{i^+}{2\sqrt{t^+}} \right) + C_s^+
\]

(A2.2)

Let the case with the following conditions be studied:

- \( C_s^+ = 1 \)
- \( C_0^+ = 0 \)

I.e. the concentration at the wall \( i^+=0 \) equals 1 and the concentration in the rest of the domain is 0 at the time \( t^+=0 \). eq. (A2.2) becomes:

\[
C^+(i^+, t^+) = 1 - \text{erf} \left( \frac{i^+}{2\sqrt{t^+}} \right)
\]

(A2.3)

This expression gives the concentration distribution for values of \( i^+ \) for a specified time \( t^+ \).
1-D diffusion in y-direction
Eq. (1.3) was implemented to examine the analytical concentration distribution in the y-direction (i=y), i.e. the concentration at the position of every y-node for a computational domain as seen in figure A2.2.

With a uniform grid with H=15 and 103 nodes in the y-direction the concentration profile was evaluated for t=5, and the following result was obtained.

Figure A2.2 Computational domain

Figure A2.3 Analytic concentration distribution

Numerical solution
The result was then going to be compared with a result obtained by using Crank Nicolson method with a TDMA solver. Since eq. (A2.1) is 1-dimensional diffusion with no convection the code had to be modified to fit for the actual problem.

1-D diffusion in y-direction
By letting the constants a_W and a_E equal zero in all the domain the code was modified to be valid for 1-dimensional unsteady diffusion in the y-direction. As seen from figure A2.3 the concentration gradient is steepest close to y^+=0. The grid was therefore made finer in that region.

Boundary and initial conditions

• Boundary 1, y^+=0: C^+=1
A further look in figure A2.3 reveals that the analytical concentration profile does not change along the y direction for \( y^* = 30 \). Hence, the boundary condition was chosen as.

- Boundary 2, \( y^* = H \)
  \[
  \left. \frac{dC^*}{dy^*} \right|_{y^* = H} = 0
  \]

- Initial condition, \( t^* = 0 \)
  \[ C^* = 0 \] for all nodes in the domain, except for boundary 1.

**Results**
The solution obtained by the numerical method is accurate, and remarkably good.

![Analytical and numerical concentration distribution](image)

**Figure A2.4** Analytical and numerical concentration distribution

![Absolute error](image)

**Figure A2.5** Absolute error

For given boundary conditions, initial conditions and a time step \( \Delta t^* = 0.1 \), the above concentration distribution was achieved numerically (plotted in the same figure as the analytical solution.). Figure A2.4 shows that the curves collapse almost perfectly and from figure A2.5 it is seen that the absolute error between the solutions is negligible.

1-D diffusion in x-direction
The same test was performed to investigate the concentration distribution for 1-dimensional diffusion in the x-direction. By letting the constants \( a_S \) and \( a_N \) equal zero and imposing the
corresponding boundary conditions an exactly equal result was obtained as for 1-D diffusion in y-direction.

**Conclusion**
The results verify that way of implementing Crank Nicolson time discretization scheme and solving the resulting set of algebraic equations with the TDMA solver is correct for the unsteady diffusion problems in the x- and y-direction using non uniform grids.
Appendix 3 - Effect on mass transfer from x-diffusion

The mass transfer depends on the concentration gradient at the wall and is defined as

\[ K^+ = L_p \int \frac{\partial C^+}{\partial y^+} \left|_{y^+ = 0} \right. \, dx^+ \].

Figure A3.1-A3.3 shows how the derivative \( \frac{\partial C^+}{\partial y^+} \left|_{y^+ = 0} \right. \) changes as moving from leading to trailing edge of the probe for Case 1 and for Case 2 where the x-diffusion is neglected. The area under the curves corresponds to the total mass transfer. The gradient has its highest value at the leading edge and decreases when moving from left to right, with the exception of the curve corresponding to Case 1 that suddenly increases at the trailing edge.

Figure A3.1 Concentration gradient at the probe, \( S^* = 5000 \)

Figure A3.2 Concentration gradient at the probes leading edge, \( S^* = 5000 \)

Figure A3.3 Concentration gradient at the probes trailing edge, \( S^* = 5000 \)

Figure A3.2 and A3.3 show a close up of the concentration gradient at the probes leading and trailing edge. The figures reveal that the concentration gradient in those regions is lower for Case 2, i.e. if the x-diffusion is neglected. Neglecting the x-diffusion gives consequently a
lower value of mass transfer. The difference is however quite small and the effect of the x-diffusion on the mass transfer becomes less and less important when increasing $S^t$.

A balance of the terms in the steady mass balance equation was also made. The purpose was to understand how the x-diffusion contributes to a higher concentration gradient at the probes leading and trailing edge and therefore gives a higher mass transfer.

**Analyzing the balance**

When plotting the balance, the terms in the steady equation were a bit reorganized.

$$\text{error} = -S^t y^+ \frac{\partial C^+}{\partial x^+} + \frac{\partial^2 C^+}{\partial y^+^2} + \frac{\partial^2 C^+}{\partial x^+^2}$$ (A3.1)

I.e. the convective term has been moved to the right hand side of the steady equation. In this way all positive terms of the right hand side acts to increase the value of the concentration $C^+$ for a certain position.

The balances in Figure A3.4 and A3.5 show that diffusion in x-direction plays a mayor role near the leading and the trailing edge of the probe. This naturally effects on the concentration near the probe surface in these regions. It is also notable that the terms change signs rapidly and discontinuously over the probe boundaries. This discontinuity is a result of the grid resolution. The grid independence test (Section 3.3) shows however that this doesn’t affect the mass transfer.

Figure A3.6 shows that for the interior points of the probe the dominant terms are the y-diffusion and the convection term.

![Figure A3.4 Balance at the leading edge of probe for the second y-node for $S^t$=5000](image)

**Figure A3.5** Balance at the trailing edge of probe for the second y-node for $S^t$=5000
The convective term was so small in the regions near the leading and trailing edge in comparison to the x- and y-diffusion so it has not been plotted in Figure A3.4 and A3.5. The concentration curve that is plotted has been scaled with a scaling factor 25000 in order to be seen. Balances for higher y-values were also made but are not included here. Those balances show that the x-diffusion term has the same behaviour at the leading and trailing edge up to a certain y-value but is negligible in the rest of the domain.

A deeper look at Figure A3.4 and A3.5 reveals that the y-diffusion term before the leading edge and after the trailing edge is positive and consequently tends to increase the concentration in those regions. The x-diffusion in the same regions is on the contrary negative and acts as a sink and therefore tends to decrease the concentration.

Physically this can be interpreted considering that the concentration is diffused towards the wall in the y-direction before the leading edge and after the trailing edge and then towards the probe by the x-diffusion term as illustrated in Figure A3.7 below.

Because of the zero mass flux boundary condition imposed on the wall the concentration can’t pass the impermeable wall and since the finite volume is conservative it has to be transported by x-diffusion towards the probe. This is the reason to the higher concentration gradient at the leading edge and the sudden increase of the concentration gradient at the trailing edge.
Appendix 4 - Reynolds decomposition

It has been investigated in previous studies how the mass transfer $K^+$ responds to a sinusoidal input signal $S^+$. The unsteady mass balance equation reads:

$$ \frac{\partial C^+}{\partial t^+} + S^+ y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial y^{+2}} + \frac{\partial^2 C^+}{\partial x^{+2}} \tag{A4.1} $$

Now define the instantaneous values $S^+$, $C^+$ and $K^+$ as sum of a time averaged term and a fluctuating term (Reynolds decomposition):

$$ S^+ = \bar{S}^+ + s^+ $$
$$ C^+ = \bar{C}^+ + c^+ $$
$$ K^+ = \bar{K}^+ + k^+ \tag{A4.2} $$

Then inserting the above decomposition (A4.2) into (A4.1) yields:

$$ \frac{\partial c^+}{\partial t^+} + \bar{S}^+ y^+ \frac{\partial C^+}{\partial x^+} + S^+ y^+ \frac{\partial c^+}{\partial x^+} + s^+ y^+ \frac{\partial c^+}{\partial x^+} = \frac{\partial^2 C^+}{\partial x^{+2}} + \frac{\partial^2 C^+}{\partial y^{+2}} + \frac{\partial^2 c^+}{\partial x^{+2}} + \frac{\partial^2 c^+}{\partial y^{+2}} \tag{A4.3} $$

Time averaging (A4.1) yields the equation for the time average value $\bar{C}^+$:

$$ \bar{S}^+ y^+ \frac{\partial \bar{C}^+}{\partial x^+} = \frac{\partial^2 \bar{C}^+}{\partial y^{+2}} + \frac{\partial^2 \bar{C}^+}{\partial x^{+2}} \tag{A4.4} $$

Subtracting the time averaged eq. (A4.4) from (A4.3) yields the equation for the fluctuating property $c^+$:

$$ \frac{\partial c^+}{\partial t^+} + \bar{S}^+ y^+ \frac{\partial C^+}{\partial x^+} + s^+ y^+ \frac{\partial c^+}{\partial x^+} - y^+ \frac{\partial s^+ c^+}{\partial x^+} = \frac{\partial^2 c^+}{\partial x^{+2}} + \frac{\partial^2 c^+}{\partial y^{+2}} \tag{A4.5} $$

Ling (1962) has studied the effects of the axial diffusion term, and has concluded that it may be neglected when $S^+>5000$ (Or in other words; the forced convection is large enough to let the diffusion in the x-direction $\frac{\partial^2 C^+}{\partial x^{+2}}$, be neglected).

For small amplitude fluctuations $s^+<<S^+$ it has been shown that the quadratic terms (underscored with two lines in (A4.5)) are negligible (Fortuna and Hanratty, 1966).

Equations (A4.4) and (A4.5) then read:

$$ \bar{S}^+ y^+ \frac{\partial \bar{C}^+}{\partial x^+} = \frac{\partial^2 \bar{C}^+}{\partial y^{+2}} \tag{A4.4'} $$

$$ \frac{\partial c^+}{\partial t^+} + \bar{S}^+ y^+ \frac{\partial C^+}{\partial x^+} + s^+ y^+ \frac{\partial C^+}{\partial x^+} = \frac{\partial^2 c^+}{\partial y^{+2}} \tag{A4.5'} $$

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The time average equation Eq. (A4.4’) and the equation for the fluctuating property Eq. (A4.5’) are coupled and can be solved numerically. When a time averaged and fluctuating concentration fields are obtained the mass transfer can be calculated by the following relations.

\[
\overline{K^+} = L_p \int_{y''=0} \frac{\partial C^+}{\partial y'} \, dx^+
\]  
(A4.6)

\[
k^+ = L_p \int_{y''=0} \frac{\partial c^+}{\partial y'} \, dx^+
\]  
(A4.7)

The frequency response reported by Py (1990) has been achieved solving the mass balance equation in this manner. This frequency response is valid for small amplitude fluctuations and for \(S^+>5000\).

For the time average equation (A4.4’) there is also an analytical solution and the mass transfer can be calculated with the analytical expression:

\[
\overline{K^+} = 0.807 S^{+0.7}
\]  
(A4.8)
Appendix 5 – Matlab code

A5.1 Pre-processor

clear all;
close all;
K_old=10000000;

%%% Defining geometry and in data
%%% All expressed as dimensionless coordinates

delta_t=10^-6;  %length of timestep
S=5000 %velocity gradient, for steady state code
CB=1; %bulk concentration;
Lf=0.5; %Length upstream of probe
Lp=1; %Probe length
Lr=0.5; %Length downstream of probe
L=Lf+Lp+Lr; %Length of the domain
H=0.5; %Height of the domain

N_iLf=80;
N_iLp=160; %Cells in the i, or x direction for domain Li
N_iLr=80;
N_im1Lf=N_iLf+1;
N_im1Lp=N_iLf+N_iLp+1;
N_im1Lr=N_iLf+N_iLp+N_iLr+1;

N_first=N_im1Lf+1;
N_last=N_im1Lp;

N_i=N_iLf+N_iLp+N_iLr; %cells in the i, or x direction
N_j=80; %Cells in the j, or y direction
N_im1=N_i+1; %gridpoints in i
N_jm1=N_j+1; %gridpoints in j
N_inode=N_i+2; %nodes in i
N_jnode=N_j+2; %nodes in j

x_grid=zeros(N_im1,N_jm1);
y_grid=zeros(N_im1,N_jm1);

%--------------------generate grid---------------------------

%Domain Lf

xLf=zeros(N_im1Lf,1);
xroofLf=zeros(N_im1Lf,1);
betaLf=1.2;
for i=1:N_im1Lf
    xroofLf(i)=(i-1)/N_iLf;
    xLf(i)=Lf-Lf*(betaLf+1)-(betaLf-1)*((betaLf+1)/(betaLf-1))^(1-xroofLf(i)))/(((betaLf+1)/(betaLf-1))^(1-xroofLf(i)));
end

%%% Tannehill p 249 equ 5-216
end
xLf=flipud(xLf);

%Domain Lp

xLp=zeros(N_iLp+1,1);
xroofLp=zeros(N_iLp+1,1);
betalp=1.2;
alfalp=0.5;
for i=1:N_iLp+1
    xroofLp(i)=(i-1)/N_iLp;
    term1=betalp+2*alfalp;
    term2=betalp+1;
    term3=betalp-1;
    term4=xroofLp(i)-alfalp;
    term5=1-alfalp;
    term6=-betalp+2*alfalp;
    term7=2*alfalp+1;
    xLp(i)=Lp*((term1*((term2/term3)^(term4/term5))+term6)/(term7*(1+(term2/term3)^(term4/term5)))); %Tannehill p 250 equ 5-216
end
xLp=xLp+Lf;

%Domain Lr

xLr=zeros(N_iLr+1,1);
xroofLr=zeros(N_iLr+1,1);
betalr=1.2;
for i=1:N_iLr+1
    xroofLr(i)=(i-1)/N_iLr;
    xLr(i)=Lr*((betalr+1)-(betalr-1)*((betalr+1)/(betalr-1))^(1-xroofLr(i)))/(((betalr+1)/(betalr-1))^(1-xroofLr(i))+(1-xroofLr(i)))+1)); %Tannehill p 249 equ 5-216
end
xLr=xLr+Lf+Lp;

%generate x_grid

for j=1:N_jm1
    for i=1:N_im1Lf
        x_grid(i,j)=xLf(i);
    end
    for i=N_im1Lf:N_im1Lp
        x_grid(i,j)=xLp(i-N_im1Lf+1);
    end
    for i=N_im1Lp:N_im1Lr
        x_grid(i,j)=xLr(i-N_im1Lp+1);
    end
end

%generate y-grid
y=zeros(1,N_jm1);
yroof=zeros(1,N_jm1);
beta=1.1;
y(N_jm1)=H;
for i=1:N_jm1
yroof(i)=(i-1)/N_j;
y(i)=H*((beta+1)-(beta-1)*((beta+1)/(beta-1))^(1-
yroof(i)))/(((beta+1)/(beta-1))^(1-yroof(i))+1); %Tannehill p
249 equ 5-216
end

for i=1:N_im1
for j=1:N_jm1
y_grid(i,j)=y(j);
end
end

%-------------------------------------------------------------
%----------------Create the position of nodes,----------------
%---------- positioned in the center of each cell-------------

x_node=zeros(N_inode,N_jnode);
y_node=zeros(N_inode,N_jnode);

for i=1:N_im1-1
for j=1:N_jm1
x_node(i+1,j)= 0.5*(x_grid(i,j)+x_grid(i+1,j));
end
end

%_x_nodes on the upper boundary
for i=1:N_inode
x_node(i,N_jnode)=x_node(i,N_jnode-1);
end

%x-nodes on the right boundary
for j=1:N_jnode;
x_node(N_inode,j)=L;
end

for j=1:N_jm1-1
for i=1:N_im1
y_node(i,j+1)=0.5*(y_grid(i,j)+y_grid(i,j+1));
end
end

%y_nodes on the right boundary
for j=1:N_jnode
    y_node(N_inode, j) = y_node(N_inode-1, j);
end

% y-nodes on the upper boundary
for i=1:N_inode
    y_node(i, N_jnode) = H;
end

% Define the Concentration matrix
C=ones(N_inode, N_jnode);

% Define the constants for the inner nodes
Dw=zeros(N_inode, N_jnode);
De=zeros(N_inode, N_jnode);
Ds=zeros(N_inode, N_jnode);
Dn=zeros(N_inode, N_jnode);
Fw=zeros(N_inode, N_jnode);
Fe=zeros(N_inode, N_jnode);
Fw_prim=zeros(N_inode, N_jnode);
Fe_prim=zeros(N_inode, N_jnode);
aW=zeros(N_inode, N_jnode);
aE=zeros(N_inode, N_jnode);
aS=zeros(N_inode, N_jnode);
aN=zeros(N_inode, N_jnode);
aP=zeros(N_inode, N_jnode);
Su=zeros(N_inode, N_jnode);
SP=zeros(N_inode, N_jnode);
delta_v=zeros(N_inode, N_jnode);

for i=2:N_inode-1
    for j=2:N_jnode-1
        Dw(i, j) = (y_grid(i-1, j) - y_grid(i-1, j-1)) / (x_node(i, j) - x_node(i-1, j));
        De(i, j) = (y_grid(i, j) - y_grid(i, j-1)) / (x_node(i+1, j) - x_node(i, j));
        Ds(i, j) = (x_grid(i, j-1) - x_grid(i-1, j-1)) / (y_node(i, j) - y_node(i, j-1));
        Dn(i, j) = (x_grid(i, j) - x_grid(i-1, j)) / (y_node(i, j+1) - y_node(i, j));
        delta_v(i, j) = (x_grid(i, j-1) - x_grid(i-1, j-1)) * (y_grid(i, j) - y_grid(i, j-1));
        aS(i, j) = Ds(i, j);
        aN(i, j) = Dn(i, j);
    end
end
\begin{align*}
Fw(i,j) &= S \cdot y_{\text{node}}(i,j) \cdot (y_{\text{grid}}(i-1,j) - y_{\text{grid}}(i-1,j-1)) \\
Fe(i,j) &= S \cdot y_{\text{node}}(i,j) \cdot (y_{\text{grid}}(i,j) - y_{\text{grid}}(i,j-1)) \\
Fw_{\text{prim}}(i,j) &= y_{\text{node}}(i,j) \cdot (y_{\text{grid}}(i-1,j) - y_{\text{grid}}(i-1,j-1)) \\
Fe_{\text{prim}}(i,j) &= y_{\text{node}}(i,j) \cdot (y_{\text{grid}}(i,j) - y_{\text{grid}}(i,j-1)) \\
\end{align*}
\end{equation}
A5.2 Solver – steady state
for i=2:N_inode-1
for j=2:N_jnode-1
aW(i,j)=max(Fw(i,j),Fw(i,j)/2+Dw(i,j));   %---hybrid scheme
aE(i,j)=max(De(i,j)-Fe(i,j)/2,0);         %---hybrid scheme
aS(i,j)=Ds(i,j);                          %---hybrid scheme
aN(i,j)=Dn(i,j);                          %---hybrid scheme
end
end

%Imposing boundary conditions:

%Node(2,2)
%Given concentration on the west boundary, dC/dy=0 on the
south boundary
i=2;
j=2;

aS(i,j)=0;
SP(i,j)=-(aW(i,j));
Su(i,j)=CB*(aW(i,j));
aW(i,j)=0;

%Node(2,3:N_jnode-2)
%Given concentration on the west boundary
for j=3:N_jnode-2
SP(i,j)=-(aW(i,j));
Su(i,j)=CB*(aW(i,j));
aW(i,j)=0;
end

%Node(2,N_jnode-1)
%Given concentration on the west boundary, given concentration
on the north boundary
i=2;
j=N_jnode-1;
aN(i,j)=0;
SP(i,j)=-aW(i,j)-Dn(i,j);
Su(i,j)=CB*(aW(i,j))+CB*Dn(i,j);
aW(i,j)=0;

%Node(3:N_inode-2,N_jnode-1)
%Given concentration on the north boundary
j=N_jnode-1;
for i=3:N_inode-2
aN(i,j)=0;
SP(i,j)=-Dn(i,j);
Su(i,j)=CB*Dn(i,j);
end
%Node(N_inode-1,N_jnode-1)
%Given concentration on the north boundary, dC/dx=0 on the east boundary
i=N_inode-1;
for j=2:N_jnode-3
aE(i,j)=0;
SP(i,j)=-Dn(i,j);
Su(i,j)=CB*Dn(i,j);
end

%Node(N_inode-1,3:N_jnode-2)
%dC/dx=0 on the east boundary
i=N_inode-1;
for j=3:N_jnode-2
aE(i,j)=0;
SP(i,j)=0;
Su(i,j)=0;
end

%Node(N_inode-1,2)
%dC/dx=0 on the east boundary, dC/dy=0 on the south boundary
i=N_inode-1;
for j=2
aE(i,j)=0;
aS(i,j)=0;
SP(i,j)=0;
Su(i,j)=0;
end

%Node(3:N_first-1,2)
%dC/dy=0 on the south boundary
j=2;
for i=3:N_first-1
aS(i,j)=0;
SP(i,j)=0;
Su(i,j)=0;
end

%Node(N_first:N_last,2)
%Given concentration on the south boundary
j=2;
for i=N_first:N_last
aS(i,j)=0;
SP(i,j)=-Ds(i,j);
Su(i,j)=0;
end

%Node(N_last+1:N_inode-2,2)
%dC/dy=0 on the south boundary
j=2;
for i=N_last+1:N_inode-2
aS(i,j)=0;
\[
\begin{align*}
SP(i,j) &= 0; \\
Su(i,j) &= 0; \\
\end{align*}
\]

%Generate aP for each node
for i=2:N_inode-1
for j=2:N_jnode-1
aP(i,j)=aW(i,j)+aE(i,j)+aS(i,j)+aN(i,j)+Fe(i,j)-Fw(i,j)-
SP(i,j);
end
end

%---Defining concentration matrix
C=ones(N_inode,N_jnode);

%----------------------------------
%-------------------------TDMA Solver-------------------------
alfa=aN;
beta=aS;
D=aP;
A=zeros(N_inode,N_jnode);
Qprim=zeros(N_inode,N_jnode);
Q=zeros(N_inode,N_jnode);
alfa_2=aE;
beta_2=aW;
D_2=aP;
A_2=zeros(N_inode,N_jnode);
Qprim_2=zeros(N_inode,N_jnode);

for n=1:10000
%----------------Sweep from west to east--------------
for j=2:N_jnode-1
for i=2:N_inode-1
Q_2(i,j)=aS(i,j)*C(i,j-1)+aN(i,j)*C(i,j+1)+Su(i,j);
A_2(i,j)=alfa_2(i,j)/(D_2(i,j)-beta_2(i,j)*A_2(i-1,j));
Qprim_2(i,j)=(beta_2(i,j)*Qprim_2(i-
1,j)+Q_2(i,j))/(D_2(i,j)-beta_2(i,j)*A_2(i-1,j));
end
for i=N_inode-1:-1:2
C(i,j)=A_2(i,j)*C(i+1,j)+Qprim_2(i,j);
end
end

end
%--------------------------------------------------------
%----------------Sweep from south to north----------------

for i=2:N_inode-1
    for j=2:N_jnode-1
        Q(i,j)=aW(i,j)*C(i-1,j)+aE(i,j)*C(i+1,j)+Su(i,j);
        A(i,j)=alfa(i,j)/(D(i,j)-beta(i,j)*A(i,j-1));
        Qprim(i,j)=(beta(i,j)*Qprim(i,j-1)+Q(i,j))/(D(i,j)-beta(i,j)*A(i,j-1));
    end
    for j=N_jnode-1:-1:2
        C(i,j)=A(i,j)*C(i,j+1)+Qprim(i,j);
    end
end
%--------------------------------------------------------

%-calculating the mass transfer Kplus
Kplus=0;
j=2;
for i=N_first:N_last
    Kplus=Kplus+C(i,j)*(x_grid(i,j)-x_grid(i-1,j))/y_node(2,2);
end
Kplus

%The solver stops when Kplus does not change between two
%iterations in space
if Kplus_old==Kplus
    break
end
Kplus_old=Kplus
end
A5.3 Solver – unsteady state

for t=1:11000  %starting iteration in time
t
f_py=1;       %frequency of the fluctuating property
%expressed in non dimensionalisation
T=t*delta_t;
Sa=5000;
f=f_py*Sa^(2/3); %converting frequency to my non
%dimensionalisation
Sf=100*sin(2*pi*f*T);
S=Sa+Sf;

for i=2:N_inode-1
for j=2:N_jnode-1
Fw(i,j)=S*Fw_prim(i,j);
Fe(i,j)=S*Fe_prim(i,j);
end
end

for i=2:N_inode-1
for j=2:N_jnode-1
aW(i,j)=max(Fw(i,j),Fw(i,j)/2+Dw(i,j));
aE(i,j)=max(De(i,j)-Fe(i,j)/2,0);
end
end

%---------------imposing boundary conditions------------------

%Node(2,2)
%Given concentration on the west boundary, dC/dy=0 on the
south boundary
i=2;
j=2;
aS(i,j)=0;
SP(i,j)=-(aW(i,j));
Su(i,j)=CB*(aW(i,j));
aW(i,j)=0;

%Node(2,3:N_jnode-2)
%Given concentration on the west boundary
i=2;
for j=3:N_jnode-2
SP(i,j)=-(aW(i,j));
Su(i,j)=CB*(aW(i,j));
aW(i,j)=0;
end

%Node(2,N_jnode-1)
% Given concentration on the west boundary, given concentration
% on the north boundary
i = 2;
j = N_jnode - 1;
aN(i, j) = 0;
SP(i, j) = -aW(i, j) - Dn(i, j);
Su(i, j) = CB*aW(i, j) + CB*Dn(i, j);
aW(i, j) = 0;

% Node (3:N_inode-2, N_jnode-1)
% Given concentration on the north boundary
j = N_jnode - 1;
for i = 3:N_inode-2
    aN(i, j) = 0;
    SP(i, j) = -Dn(i, j);
    Su(i, j) = CB*Dn(i, j);
end

% Node (N_inode-1, N_jnode-1)
% Given concentration on the north boundary, dC/dx = 0 on the
% east boundary
i = N_inode - 1;
j = N_jnode - 1;
aE(i, j) = 0;
aN(i, j) = 0;
SP(i, j) = -Dn(i, j);
Su(i, j) = CB*Dn(i, j);

% Node (N_inode-1, 3:N_jnode-2)
% dC/dx = 0 on the east boundary
i = N_inode - 1;
for j = 3:N_jnode-2
    aE(i, j) = 0;
    SP(i, j) = 0;
    Su(i, j) = 0;
end

% Node (N_inode-1, 2)
% dC/dx = 0 on the east boundary, dC/dy = 0 on the south boundary
i = N_inode - 1;
j = 2;
aE(i, j) = 0;
aS(i, j) = 0;
SP(i, j) = 0;
Su(i, j) = 0;

% Node (3:N_first-1, 2)
% dC/dy = 0 on the south boundary
j = 2;
for i = 3:N_first-1
    aS(i, j) = 0;
\[
\text{SP}(i,j)=0; \quad \text{Su}(i,j)=0; \\
\text{end}
\]

\%Node(N\_first:N\_last,2)
\%Given concentration on the south boundary
\text{j}=2;
\text{for i=N\_first:N\_last}
\text{aS}(i,j)=0;
\text{SP}(i,j)=-\text{Ds}(i,j);
\text{Su}(i,j)=0;
\text{end}

\%Node(N\_last+1:N\_inode-2,2)
\%dC/dy=0 on the south boundary
\text{j}=2;
\text{for i=N\_last+1:N\_inode-2}
\text{aS}(i,j)=0;
\text{SP}(i,j)=0;
\text{Su}(i,j)=0;
\text{end}

\%-------------------------------------------------------------
\% %Generate aP and Su2
\text{for i=2:N\_inode-1}
\text{for j=2:N\_jnode-1}
\text{aP}(i,j)=2*\text{delta}_v(i,j)/\text{delta}_t+\text{aW}(i,j)+\text{aE}(i,j)+\text{aS}(i,j)+\text{aN}(i,j)
+\text{Fe}(i,j)-\text{Fw}(i,j)-\text{SP}(i,j);
\text{Su2}(i,j)=(2*\text{delta}_v(i,j)/\text{delta}_t-\text{aW}(i,j)-\text{aE}(i,j)-\text{aS}(i,j)-
\text{aN}(i,j)-\text{Fe}(i,j)+\text{Fw}(i,j)+\text{SP}(i,j))*\text{C\_old}(i,j)+...
 +\text{aW}(i,j)*\text{C\_old}(i-1,j)...
 +\text{aE}(i,j)*\text{C\_old}(i+1,j)...
 +\text{aS}(i,j)*\text{C\_old}(i,j-1)...
 +\text{aN}(i,j)*\text{C\_old}(i,j+1)...
 +\text{Su}(i,j);
\text{end}
\text{end}

\%-----------------------------------------------------------TDMA solver------------------------------------------
\text{alfa}=\text{aN};
\text{beta}=\text{aS};
\text{D}=\text{aP};
\text{A}=\text{zeros}(\text{N\_inode},\text{N\_jnode});
\text{Q\_prim}=\text{zeros}(\text{N\_inode},\text{N\_jnode});
\text{Q}=\text{zeros}(\text{N\_inode},\text{N\_jnode});

\text{alfa\_2}=\text{aE};
\text{beta\_2}=\text{aW};
\text{D\_2}=\text{aP};
A_2=zeros(N_inode,N_jnode);
Qprim_2=zeros(N_inode,N_jnode);

for n=1:5000 %starting spatial iteration
    %----------------Sweep from west to east-----------------
    for j=2:N_jnode-1
        for i=2:N_inode-1
            Q_2(i,j)=aS(i,j)*C(i,j-1)+aN(i,j)*C(i,j+1)+Su(i,j)+Su2(i,j);
            A_2(i,j)=alfa_2(i,j)/(D_2(i,j)-beta_2(i,j)*A_2(i-1,j));
            Qprim_2(i,j)=(beta_2(i,j)*Qprim_2(i-1,j)+Q_2(i,j))/(D_2(i,j)-beta_2(i,j)*A_2(i-1,j));
        end
        for i=N_inode-1:-1:2
            C(i,j)=A_2(i,j)*C(i+1,j)+Qprim_2(i,j);
        end
        C=C_old+omega2*(C-C_old);
    end

    %----------------Sweep from south to north----------------
    for i=2:N_inode-1
        for j=2:N_jnode-1
            Q(i,j)=aW(i,j)*C(i-1,j)+aE(i,j)*C(i+1,j)+Su(i,j)+Su2(i,j);
            A(i,j)=alfa(i,j)/(D(i,j)-beta(i,j)*A(i,j-1));
            Qprim(i,j)=(beta(i,j)*Qprim(i,j-1)+Q(i,j))/(D(i,j)-beta(i,j)*A(i,j-1));
        end
        for j=N_jnode-1:-1:2
            C(i,j)=A(i,j)*C(i,j+1)+Qprim(i,j);
        end
    end
    Kplus=Kplus+C(i,j)*(x_grid(i,j)-x_grid(i-1,j))/y_node(2,2);
end

Kplus=0;
j=2;
for i=N_first:N_last
    Kplus=Kplus+C(i,j)*(x_grid(i,j)-x_grid(i-1,j))/y_node(2,2);
end
if K_old==Kplus
break
end
K_old=Kplus;

end %spatial iteration

C_old=C;

Kplus_t(t+1)=Kplus; %saving the mass transfer Kplus for each
%time step

end %time iteration

%-------------------------------------------------------------