Chapter II

Theoretical Considerations

It has been mentioned that the transport of moisture within a porous media is proportional to its concentration gradient if influence of temperature and pressure gradients can be neglected (W.J.A.H. Schoeber, 1976). This simplification allows the phenomenon to be described by a diffusion equation with a diffusion coefficient which varies with water concentration. The measurement of the concentration dependence of this diffusion coefficient has been the object of several studies (S. Yamamoto, M Hoshika, Y. Sano, 1984; M. Suzuki, S. Maeda,1978; V.T.Karathanos, G.Villalobos, G.D. Saravacos,1990). Among concentration dependence of diffusion coefficients mentioned in the above references are the linear concentration dependence, the exponential concentration dependence, and the power-law concentration dependence.

The following will be a derivation of the equations describing moisture diffusion in a porous media where moisture concentration alone will be the major driving force. The boundary conditions will relate to a water saturated bed of porous media suddenly exposed at the top to ambient air at varying conditions. The system will operate under isothermal conditions.

The Diffusion Equation

The derivation of the diffusion equation may be done by a differential moisture balance in a slab of porous media as follows

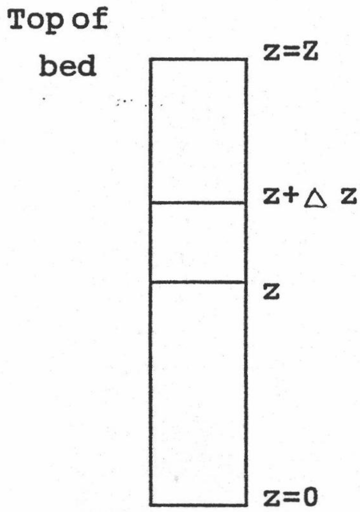

Figure 2.1 Schematic representation of a column filled with a porous media

The mass balance on a slab in a column between position $z = z$ and $z = z+\Delta z$ can be written as

rate of mass in - rate of mass out = rate of mass accumulation

$$-AD\frac{\partial w_w}{\partial z}\Big|_z + AD\frac{\partial w_w}{\partial z}\Big|_{z+\Delta z} = A\Delta z\frac{\partial w_w}{\partial t} \qquad (2-1)$$

Dividing by $A\Delta z$ and taking the limit as $\Delta z \rightarrow 0$ gives

$$\frac{\partial}{\partial z} D \frac{\partial w}{\partial z} = \frac{\partial w}{\partial t} \tag{2-2}$$

But $\dfrac{w}{\text{dry weight}} = \dfrac{\text{wet weight-dry weight}}{\text{dry weight}} = m$

$$\frac{\partial w}{\partial z} = \text{dry weight} \frac{\partial m}{\partial z} \tag{2-3}$$

$$\frac{\partial w}{\partial t} = \text{dry weight} \frac{\partial m}{\partial t} \tag{2-4}$$

$$\frac{\partial}{\partial z} D \times \frac{1}{\text{dry weight}} \frac{\partial w}{\partial z} = \frac{1}{\text{dry weight}} \frac{\partial w}{\partial t} \tag{2-5}$$

From equation (2-3) to (2-5) we obtain

$$\frac{\partial}{\partial z} D \frac{\partial m}{\partial z} = \frac{\partial m}{\partial t} \tag{2-6}$$

Let D be dimensionless : D_r and D_r depends on concentration.

We finally obtain

$$\frac{\partial}{\partial z} D_r(m) \frac{\partial m}{\partial z} = \frac{\partial m}{\partial t} \tag{2-7}$$

We have the following initial condition

$$m(t=0,z) = m_0(z) \tag{2-8}$$

and the following boundary conditions

$$\frac{\partial m}{\partial z}(t,z=0) = 0$$

$$m(t,z=z) = m_s(z) \qquad (2-9)$$

1. Placing the equations in a finite difference form.

We write m(t,z) in the form of m(i,j) where i refers to time increments and j refers to (depth) position within the column.

The partial differential equation then becomes

$$\frac{\partial}{\partial z} D_r(m) \frac{\partial m}{\partial z} = \frac{\partial m}{\partial t} \qquad (2-10)$$

$$D_r(m)\frac{\partial^2 m}{\partial z^2} + \frac{dD_r(m)}{dm}\left(\frac{\partial m}{\partial z}\right)^2 = \left(\frac{\partial m}{\partial t}\right) \qquad (2-11)$$

We illustrate the finite difference method (Finlayson,1980) by application to equation 2-7, and let

$$m_j(t) = m(z_j,t) \quad .$$

$$\frac{dm_j}{\partial t} = \frac{1}{\Delta z^2}[D_r(m_{j+1/2})(m_{j+1} - m_j) - D_r(m_{j-1/2})(m_j - m_{j+1})] \qquad (2-12)$$

Application of a simple Euler method gives

$$\frac{m(i+1,j) - m(i,j)}{\Delta t} = \frac{1}{\Delta z^2}[D_r(m_{i,j+1/2})(m(i,j+1) - m(i,j)) - D_r(m_{i,j-1/2})(m(i,j) - m(i,j-1))] \qquad (2-13)$$

where $m(i,j) = m(t_i, z_j)$

We expand the equation in a Taylor series and use a truncation error,(Finlayson,1980) and the scheme is second-order provided.

$$\frac{1}{2}[D_r(m_{i,j+1/2}) + D_r(m_{i,j-1/2})] = D_r(m_{i,j}) + 0(\Delta z^2) \tag{2-14}$$

Where $0(\Delta z^2)$ is the truncation error.

If we let D be constant for each interval then

$$\begin{aligned}\frac{m(i+1,j)-m(i,j)}{\Delta t} &= \frac{dm(i,j)}{dt} \\ &= \frac{D_r(m_{i,j})}{\Delta z^2}(m(i,j+1)-2m(i,j)+m(i,j-1)\end{aligned} \tag{2-15}$$

As $D_r(m)$ may be expressed as either $D_r = am+(1-a)$ or $D_r = \exp[a(m-1)]$ or $D_r = m^a$

The boundary conditions become

$$\begin{aligned} m(0,j) &= m_0(j) \\ m(t,j=N_d+1) &= m_s \end{aligned} \tag{2-16}$$

Where N_d = number of discretizations.

2. The computational subroutine to integrate the equation

It was decided to use the Crank Nicolson method based on an iterative search method for the i+1 row (time interval). We divide the column into N_{d+1} parts(m_j). Knowing m(0,j) being the initial condition we seek the value for row number 1 or m(i,j), we need to assume this i=1 row first, then compute the elements of the row i=1 from point $j=N_d$ to point j=0 iteratively. This method is based on solving the N_d-1 matrix

Calculation of the diffusion equation.

1. Calculation of the main equation of the Crank - Nicolson Method

Starting with the following equation.

$$\left(\frac{\partial m}{\partial t}\right) = D_r(m)\frac{\partial^2 m}{\partial z^2} \qquad (2\text{-}17)$$

We assume point E as the half time increment

m(i,j-1)	m(i,j)	m(i,j+1)
	• A	
	• E	
m(i+1,j-1)	m(i+1,j)	m(i+1,j+1)
	• D	

$$\left.\frac{\partial m}{\partial t}\right|_E = \frac{m(i+1,j)-m(i,j)}{\Delta t} \tag{2-18}$$

and

$$\left.\frac{\partial^2 m}{\partial t^2}\right|_E = \frac{1}{2}\left(\left.\frac{\partial^2 m}{\partial t^2}\right|_A + \left.\frac{\partial^2 m}{\partial t^2}\right|_D\right) \tag{2-19}$$

equation (2-17) then becomes

$$\frac{m(i+1,j)-m(i,j)}{\Delta t} = D_r(m_{i,j})\frac{1}{2}\frac{1}{\Delta z^2}[m(i,j-1)-2m(i,j) + m(i,j+1)+m(i+1,j+1)-2m(i+1,j) + m(i+1,j+1)] \tag{2-20}$$

$$\text{Let } M = \frac{D_r(m_{i,j})\Delta t}{\Delta z^2}$$ we rewrite

$$(1+M)m(i+1,j) = (1-M)m(i,j) + \frac{1}{2}M(m(i,j+1)+m(i,j-1)) + \frac{1}{2}M(m(i+1,j+1)+m(i+1,j+1)) \tag{2-21}$$

Defining a new working array F(i,j) (which we know) as follows

$$(1+M)F(i,j) = (1-M)m(i,j)\frac{1}{2}M(m(i,j+1)+m(i,j-1)) \tag{2-22}$$

We rewrite

$$m(i+1,j) = F(i,j) + \frac{M}{2(1+M)}(m(i+1,j+1)+m(i+1,j-1)) \tag{2-23}$$

Which is the equation that is to be used for the calculation.

2. Development of the computer program in the C-language

There are several functions we want the progame to do. Firstly the program calls in the initial and boundary conditions and then we can create a concentration profile at various points along the column every hour.

Then we need a program that can sum the square of the differences between the experimental points and points obtained from the first program. We need a subroutine for the form of the D_r equation.

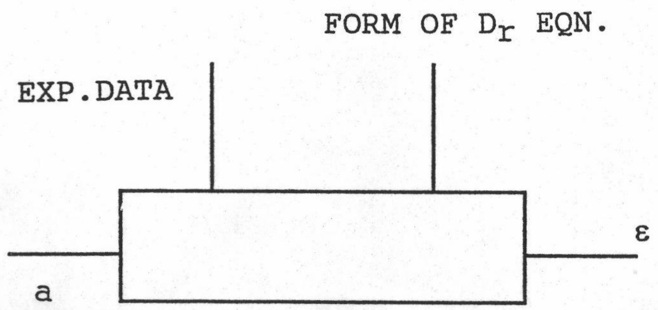

Figure 2.2 computation process

a is a parameter of the D_r Equation, ε is the criteria between experimental data and computed value.