Pollutant Transport Theory

Contaminant Flux

Transport of materials is quantified in terms of flux density or flux. Flux density is the amount of material that passes a point in space per unit area per unit time. Flux is a vector quantity with magnitude and direction. Flux vectors point in the direction of net material motion and their magnitude indicates the rate of motion in that direction.

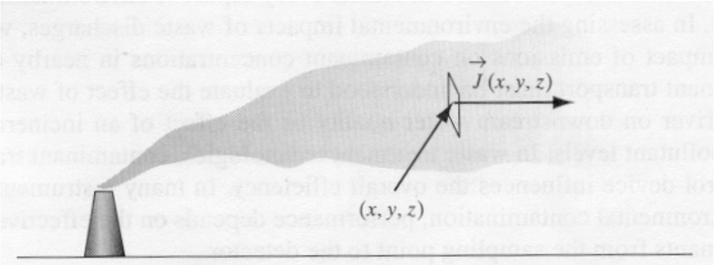


Figure 1. Flux Vector (from:)

Figure 1 depicts how a flux vector is defined. Imagine a frame centered at *(x,y,z)*, oriented perpendicular to the plume time average flow line. The mass of pollutant that passes through this frame per unit time divided by the area of the frame is called the pollutant mass flux. The amount of fluid momentum passing through the frame would be called the momentum flux. Any quantity can be defined in terms of its flux although mass, energy, and momentum are the most common quantities studied in engineering.

Advection

Advection (convection) is the transport of dissolved or suspended material by motion of the host fluid. The prediction of the direction and amount of material transported requires knowledge of the fluid velocity field (the velocity of a fluid particle).

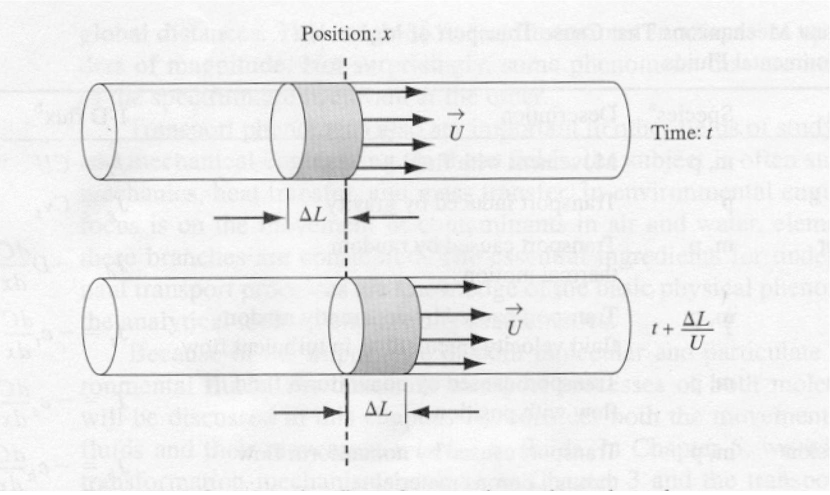


Figure 2: Labeled Fluid Parcel

Figure 2 depicts the flow of a labeled fluid in a tube. One can use the sketch to define various useful properties of the labeled fluid portion as listed.

Property	Expression
Mass of labeled fluid	$m = \rho A \Delta L$
Mass of tracer	$m = C A \Delta L$
Distance traveled by leading (trailing edge)	$x = \Delta L$
Time required to travel distance	$time = \Delta t$
Velocity of leading edge	$u = \frac{x}{time} = \frac{\Delta L}{\Delta t}$
Mass flow through circular frame	$m = \rho A \Delta L$
Tracer flow through circular frame	$m = C A \Delta L$
Mass through circular frame/unit time	$\frac{m}{time} = \frac{\rho A \Delta L}{\Delta t}$

Tracer through circular frame/unit time

$$\frac{m}{time} = \frac{CA\Delta L}{\Delta t}$$

Fluid mass flux

$$J = \frac{\rho UA}{A} = \rho \frac{Q}{A} = \rho U$$

Tracer mass flux

$$J = \frac{CUA}{A} = C\frac{Q}{A} = CU$$

The advective flux is the product of the quantity of interest (in this case mass of either host fluid or tracer) and the velocity term. Typically the mean section velocity is used (pipe flow, open channel flow) because fine scale resolution of the velocity field is impossible. In porous media, the pore velocity or average linear velocity is used.

Advection calculations usually use mean section velocity based on discharge measurements.

Discharge is the volume rate of flow in a fluid system. It has dimensions of length^3/time.

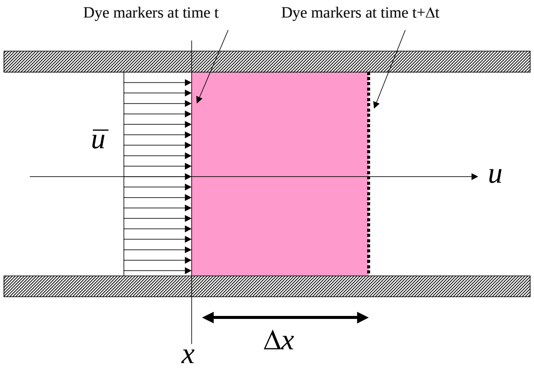


Figure 3: Mean Section Velocity - Uniform Flow Across Section

The figure is a schematic of a conduit completely filled with fluid. Dye markers are placed at location x at some time t. A short period of time later, the position of the dye markers has moved to the location shown on the diagram. The product of the area of the conduit and the distance swept by the dye markers is a volume. The ratio of this volume and time it takes for this volume to be defined is called the volumetric flow rate.

In mathematical terms, the area of the conduit is A. The volume of fluid that passed x in the time interval Δt is $\Delta x A$.

The volumetric flow rate is then

$$Q = \frac{V}{\Delta t} = \frac{\Delta x}{\Delta t} A$$

In the limit this flow rate is defined in terms of the mean section velocity, $Q = \bar{u} A$.

If the velocity varies across the section, the mean sectional velocity is found by integration.

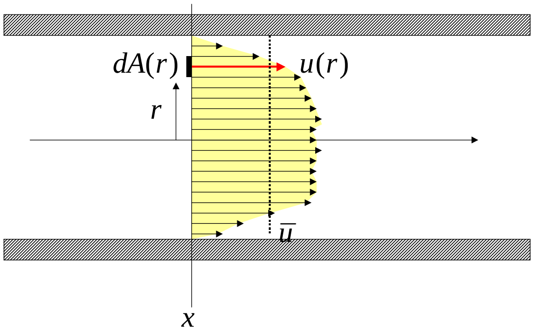


Figure 4: Mean Section Velocity - Non-Uniform Flow Across Section

From calculus we define the differential increment of discharge as, $dQ = udA$. Integration of all the differental elements is expressed as, $\int dQ = \int udA$. From the conceptual definition of average section velocity we can compute its value as the ratio of these two integrals,

$$\bar{u} = \frac{\int u dA}{\int dQ}$$

Observe that $Q = \bar{u}A$ is perpendicular to u. For an arbitrary orientation one must compute the scalar product of the velocity vector and the area vector, as depicted in Figure 3.

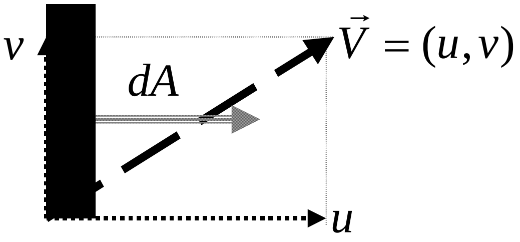
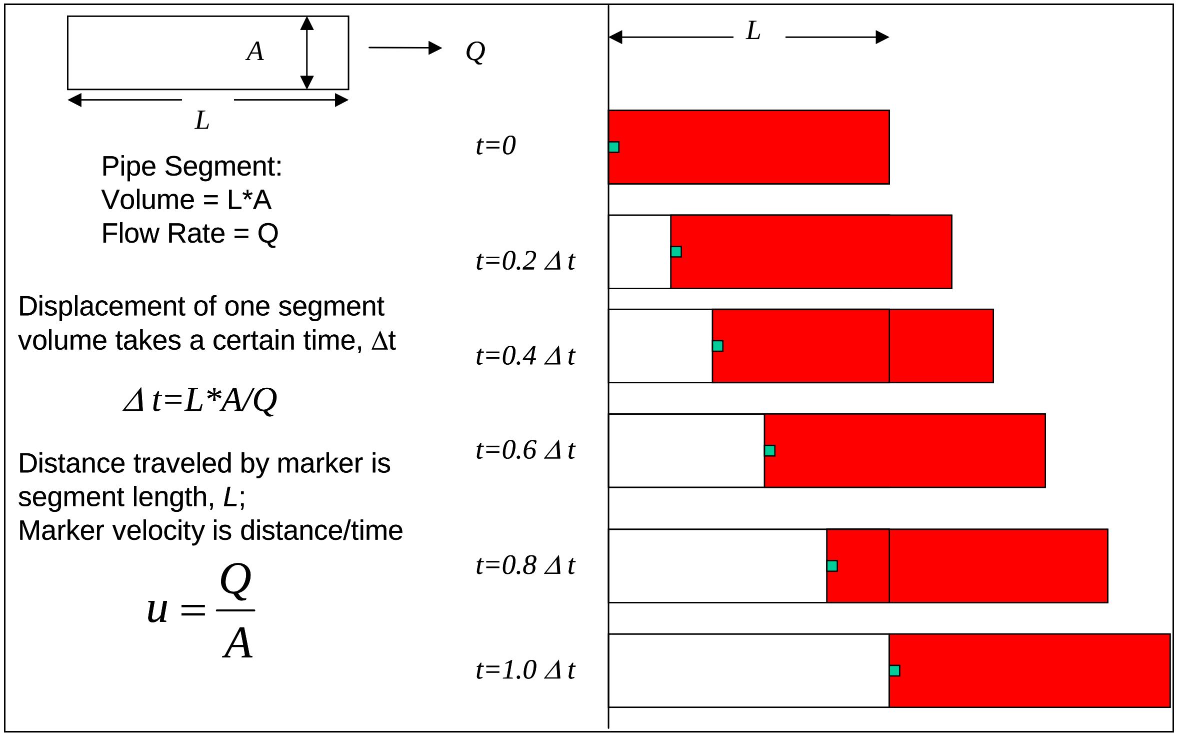


Figure 5: Non-Colinear Velocity and Area Vectors

$$Q = \int \vec{V} \bullet dA = \int u \bullet dA_x + \int v \bullet dA_y$$



Pipe Segment:
Volume = L*A
Flow Rate = Q

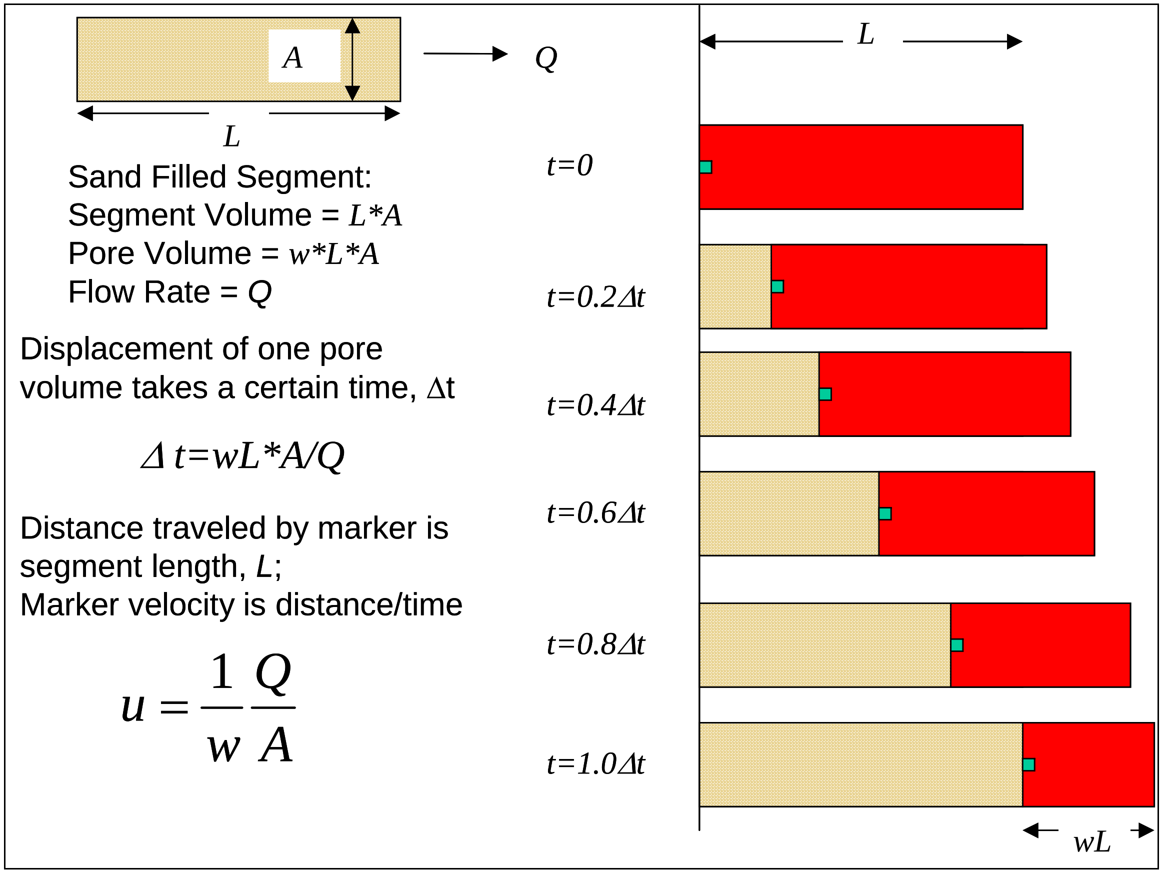
Displacement of one segment volume takes a certain time, Δt

$$\Delta t = L*A/Q$$

Distance traveled by marker is segment length, *L*;
Marker velocity is distance/time

$$u = \frac{Q}{A}$$

Figure 6: Mean Section Velocity



Sand Filled Segment:
Segment Volume = $L*A$
Pore Volume = $w*L*A$
Flow Rate = Q

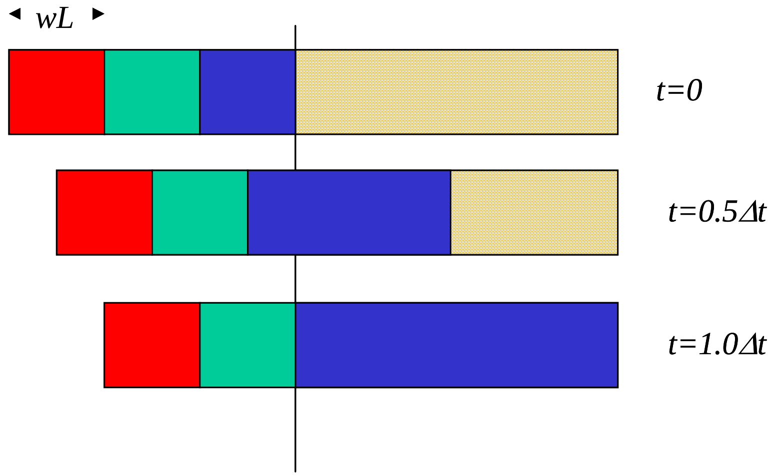
Displacement of one pore volume takes a certain time, Δt

$$\Delta t = wL*A/Q$$

Distance traveled by marker is segment length, L;
Marker velocity is distance/time

$$u = \frac{1}{w}\frac{Q}{A}$$

Figure 7: Average Linear Velocity



Suppose one “blue” pore volume enters the sand pack.

The mass of “blue” per unit volume is the concentration of blue.

Let one pore volume enter the sand pack.

Total mass of blue in the pore volume is the concentration*fluid volume

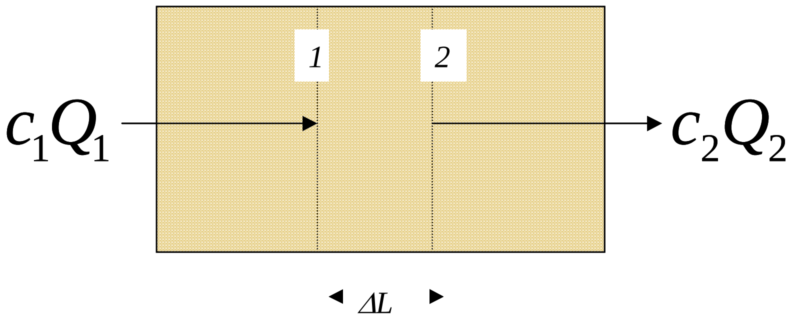
$$M_{blue} = wALC_{blue}$$

Rate of blue entering the sand pack is mass/time

$$\frac{M_{blue}}{\Delta t} = \frac{wALC_{blue}Q}{wAL} = c_{blue}Q$$

Figure 8: Mass Flux (Porous Flow)

Now consider a small portion of the sand pack.



<u>Mass flow into segment</u>. <u>Mass flow out of segment</u>. <u>Rate of accumulation in segment</u>.

$$c_1Q_1 \quad + \quad c_2Q_2 \quad = \quad \frac{\partial}{\partial t}\left[cwA\Delta L\right]$$

Figure 9: Mass Balance

For a non-deforming medium this mass balance is expressed as:

$$\frac{c_1Q_1 - c_2Q_2}{wA\Delta L} = \frac{\partial c}{\partial t}$$

Substituting the definition of average linear velocity:

$$\frac{c_1u_1 - c_2u_2}{\Delta L} = \frac{\partial c}{\partial t}$$

Taking the limit as ΔL vanishes produces the fundamental equation governing convective transport.

$$-\frac{\partial(uc)}{\partial L} = \frac{\partial c}{\partial t}$$

Figure 10: Balance Equations

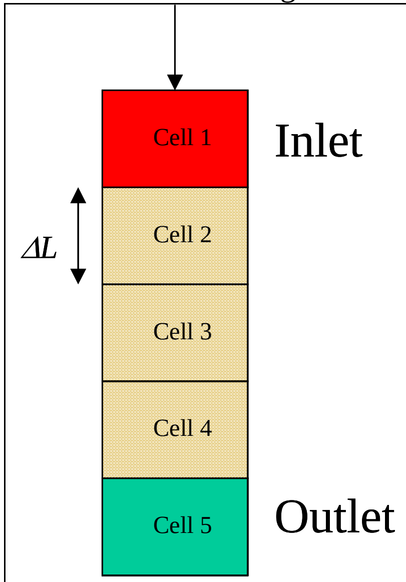
$$-\frac{\partial(uc)}{\partial x}-\frac{\partial(vc)}{\partial y}-\frac{\partial(wc)}{\partial z}=\frac{\partial c}{\partial t}$$

or

$$\frac{\partial c}{\partial t}=-div(\vec{U}c)$$

- Observe the obvious dependence on the velocity field *(u,v,w).*
- In order to compute any mass fluxes we must first determine the velocity values in the domain of interest.

Figure 11: 3D Generalization



Suppose at t=0 the concentration in the inlet cell is Co. We want to determine the concentration in the porous medium at future times.

We will assume the pore velocity is identical throughout the column.

A simple modeling approach is to treat each cell as completely mixed. This means that the concentration at the cell exit is identical to the concentration in the cell.

Figure 12: Cell Balance Model (Cascade Reactors)

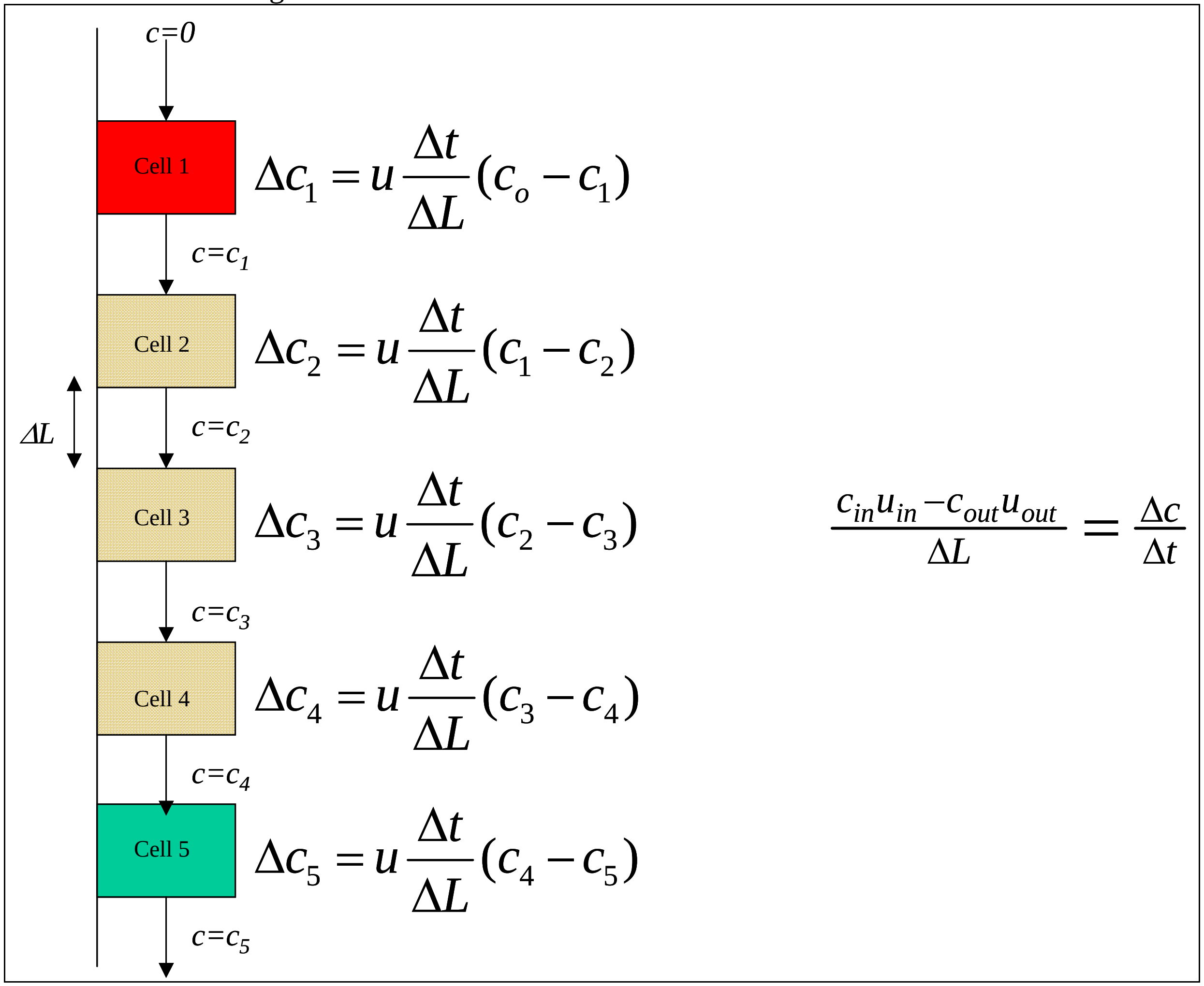
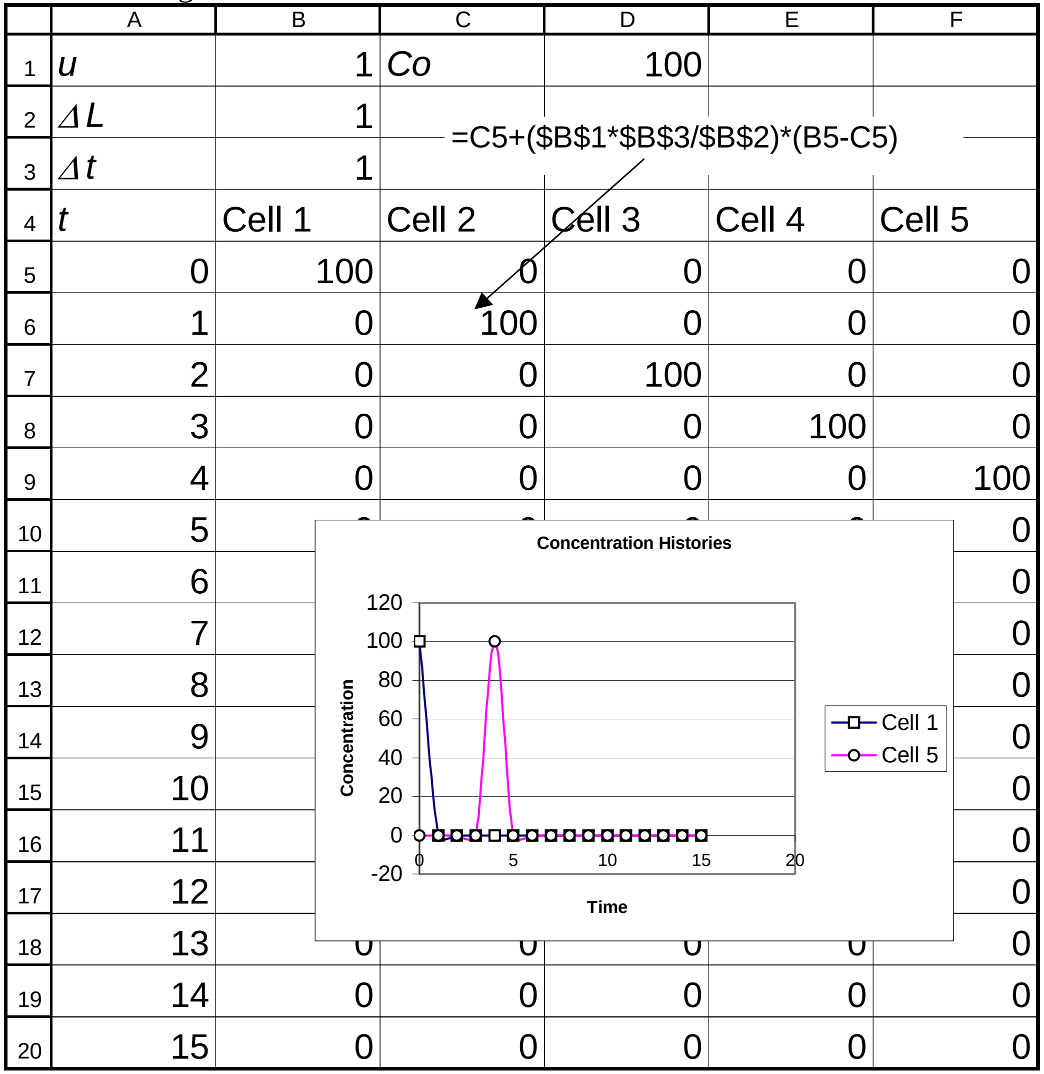


Figure 13: Difference Equations



=C5+($B$1*$B$3/$B$2)*(B5-C5)

	A	B	C	D	E	F
1	*u*	1	*Co*	100		
2	*ΔL*	1				
3	*Δt*	1				
4	*t*	Cell 1	Cell 2	Cell 3	Cell 4	Cell 5
5	0	100	0	0	0	0
6	1	0	100	0	0	0
7	2	0	0	100	0	0
8	3	0	0	0	100	0
9	4	0	0	0	0	100
10	5	[illegible]	[illegible]	[illegible]	[illegible]	0
11	6	[illegible]	[illegible]	[illegible]	[illegible]	0
12	7	[illegible]	[illegible]	[illegible]	[illegible]	0
13	8	[illegible]	[illegible]	[illegible]	[illegible]	0
14	9	[illegible]	[illegible]	[illegible]	[illegible]	0
15	10	[illegible]	[illegible]	[illegible]	[illegible]	0
16	11	[illegible]	[illegible]	[illegible]	[illegible]	0
17	12	[illegible]	[illegible]	[illegible]	[illegible]	0
18	13	0	0	0	0	0
19	14	0	0	0	0	0
20	15	0	0	0	0	0

Figure 14: Spreadsheet Solution