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1

Introduction

This chapter provides an overview of the course. The course is technically demanding so students are advised to attend lectures regularly, solve the assignments, compare it with the solutions posted bi-weekly and engage in class discussions.

1.1. Learning points

The course is composed of the following topics:

1. Lakes and rivers: understanding how to make a mass balance of dissolved substances and how to build your own model such as Rhine Alarm Model.
2. Estuaries: salinity intrusion modeling in estuaries, making use of analytical solutions that can be directly linked to ecological relationships.
3. Coupled environmental quality and economic growth models in context of sustainable development.

1.2. Lecturers

Dr. Saket Pande is the course manager with expertise in hydrology and water economics and covers Module 1 and 3. He sits in room CiTG 4.81. Saket has a B.Tech in Civil and Environmental Engineering from Indian Institute of Technology Delhi, India and Ph.D. in Hydrology and Water Resource Management from Utah State University, Logan-UT, USA.

Prof. Dr. ir. H.H.G. Savenije is the instructor on the module salinity in estuaries.

1.3. Why Environmental Modeling?: Two examples

The 2030 Agenda for Sustainable Development of United Nations is built on 3 pillars of social, economic and environment sustainability of a growing planet. Water is a key cross-cutting theme across the goals and the impact of growing economic and social aspiration on the water quality of surface can not be ignored. The modeling of water quality and how it interacts with economic systems is key to understanding sustainable development and to intellectually participate in debates on development.

For example for sustainable cities, life on land and below water one needs to characterize quality of surface water bodies. Modeling, as a tool, is needed to extend observations, e.g. EU Water Framework Directive and to establish spatially distributed reference values.

Modeling enable us to assess susceptibility of surface water to anthropogenic (human) pressure, such as those coming from point source / diffuse pollution, intentional (waste water) or not (e.g. agriculture) or (Semi-)natural processes (e.g. salinization). All these inherently contribute to responsible consumption and production, e.g. in context of circular economy and nature based solutions to used water.

Accidents and disaster prevention is not only important for good health and well-being but by designing sampling schemes and action plans, one can contribute to decent work, economic growth, industry, innovation and infrastructure.



Figure 1.1: The sustainable development goals where water is the key cross-cutter. Source: <http://www.un.org/sustainabledevelopment/sustainable-development-goals/>

1.3.1. Water Quality Modeling preempts cancer

Following (Figure 1.2) is a clear example of how water quality modeling enables us to understand the spatial extent of potentially carcinogenic effects of what otherwise may sound like a safe technology to harness our natural resources, i.e. hydraulic fracturing. Water at high pressure is pumped into the wells to push out natural gas. But alongside, heavy metals are also dislodged and carried out by the same water. Heavy metals are not removed by waste-water treatment plants and enter the local urban cycle.

In order to safeguard well-being of local communities, a modeling exercise may start with the source of pollutants, i.e. point sources, and location of local communities. Then how pollutants are transported from sources to local communities can be understood by modeling the transport of radio-active pollutants through surface and sub-surface water bodies.

1.3.2. Coupled environment quality and economic growth

We prefer better environmental quality but also better livelihood, more income or better economy. Often there is a trade-off between them. Water quality modeling guides us in terms of interventions needed for sustainable living. For example, the challenge posed by agriculture productivity driven fertilizer application can be converted into opportunity as the nutrients in the used water can be recycled in context of circular economy to meet ever increased demand for agricultural inputs.

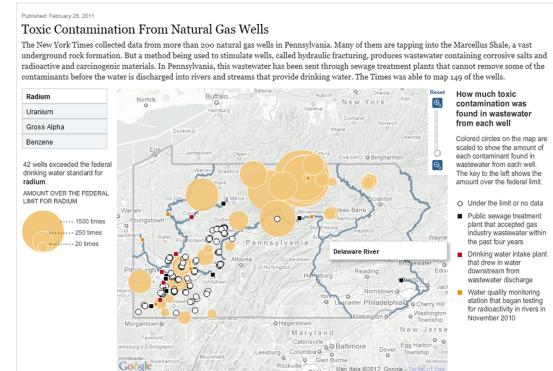


Figure 1.2: Risk assessment: how hydraulic fracturing carcinogenic effects propagates downstream.

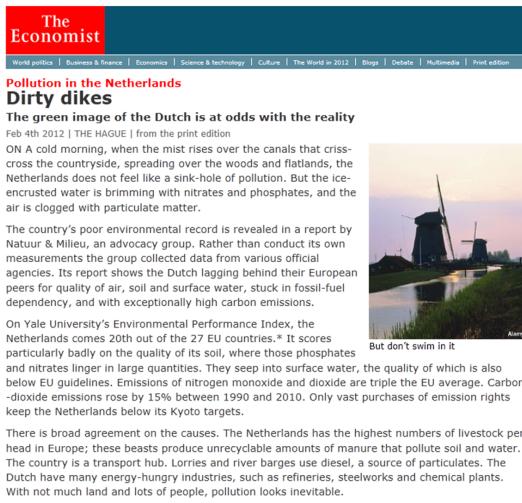


Figure 1.3: Dont Swim in it: water bodies in Netherlands contain heavy doses of industrial and agricultural nutrients. Source: <http://www.economist.com/node/21546053>

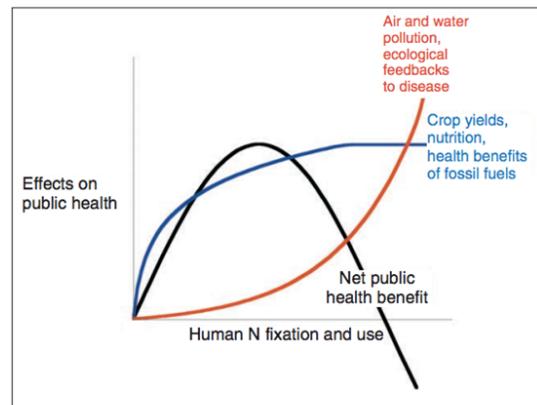


Figure 1. Conceptual model of the overall net public health effects of increasing human fixation and use of atmospheric N_2 . As human N_2 fixation and use rises, the positive effects of N on crop growth, food production, and overall nutrition peak (and potentially begin to decrease). A similar pattern appears in the public health benefits of increasing fossil fuel use associated with better city infrastructure and transportation. In contrast, rising N inputs create exponential increases in losses of N to air and water, deposition to natural ecosystems, and potential feedbacks between rising N availability and the ecological dynamics of environmentally-harbored diseases.

Figure 1.4: Peak in net public health benefit. Source: onehealtheducation.blogspot.com

1.4. Building water quality models

Completely mixed systems are those wherein the concentration of pollutants does not change within the surface body under consideration. Modeling is relatively simple, essentially as mass balance of what goes into the system and what comes out of the system, which then is reflected in the change in concentration of pollutants over time. Transformation processes that may be chemical, physical, or biological are also part of the mass balance that take the pollutants out of the equation.

Concentration of pollutants within incompletely mixed systems vary from point to point within a surface water body. For example, consider stagnant zones of a river where concentration of a substance is different from other parts of the river. Two things need consideration, 1) transport of substances within a water body, i.e. transport with the flow (advection) and mixing with the water flow (diffusion or dispersion) and 2) transformation due to chemical or biological reactions.

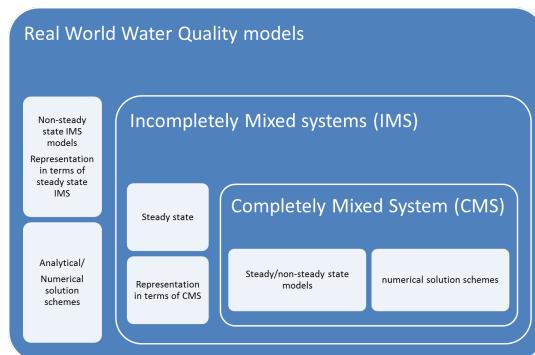


Figure 1.5: Water Quality Modeling of surface bodies: Synopsis.

The course takes a hierarchical approach to building such technical water quality model (see Fig 1.5). The concepts are explained layer by layer, with complexity of models increasing over time.

Coupled water-quality and population growth models take a higher level view and aims to keep

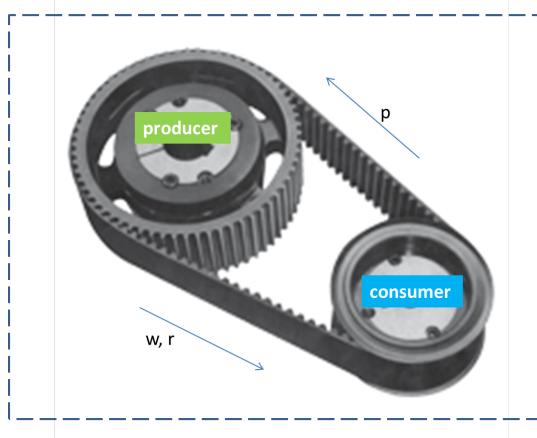


Figure 1.6: Human societies are composed of producers and consumers who depend on each other, and as the society evolves, they generate pollution that may in return restrict growth potential.

various components of such a model at lower level of complexity such that the complexity of interaction between the water and the human system can be explored in greater detail. Humans affect water quality by their need to produce goods and services that satisfy the needs of a growing population. The understanding of coupled human-water quality system dynamics requires an equal attention to the human dynamics. This course pays attention to some of the needed fundamentals. Following are the topics covered:

1. Constrained/unconstrained optimization
2. Why agents consume?-utility maximization
3. How producers produce?-profit maximization
4. How prices of goods appear?
5. Conceptualization of a society – overlapping generations model

By doing so, one is able to answer the following questions towards the end of the course:

1. How can we build low order models of economies or societies realistically?
2. Do we need models that determine how environment and economic growth shape each other as societies evolve over generations?
3. where scope for investment in environment and economic growth is possible?

2

Completely mixed systems

This chapter deals with completely mixed systems. Lakes and rivers that are completely mixed with, e.g. salt, have concentration of such substances invariant within their system boundaries. The mass balances of water and the substances are needed to be solved.

2.1. Fundamental Equation

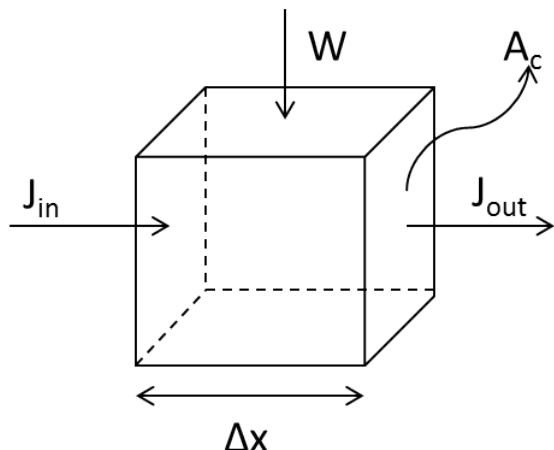


Figure 2.1: A differential element within which conservation of mass is applied.

The mass balance of water (see Figure 3.3) can be given by,

$$\frac{d\rho\Delta V}{dt} = J_{in}^\rho A_c - J_{out}^\rho A_c + W \quad (2.1)$$

While the mass balance for a substance is given by,

$$\frac{dc\Delta V}{dt} = J_{in}^c A_c - J_{out}^c A_c + W. \quad (2.2)$$

Here,

ΔV	Volume of the differential element [L^3]
J_{in}^*	incoming mass flux rate of * [ML^{-2}/T]
J_{out}^*	incoming mass flux rate of * [ML^{-2}/T]
A_c	cross sectional area perpendicular to the flux rates
Δx	length of the differential element [L]
c	concentration of the substance or the pollutant [ML^{-3}]
ρ	density of water

Note that the difference between the mass balance for water and pollutants is the use of water density in the former and the use of mass density in the latter. Also note that the former does not contain any reactions that are possible in the case of substance transport, hence present in the latter.

Unless otherwise specified, following assumption will be made:

Assumption 1: Water mass balance is at steady state (unless specified otherwise), i.e. $\frac{dc\Delta V}{dt} = 0 \Rightarrow J_{in}^c A_c - J_{out}^c A_c + W = 0$

Assumption 2: If we further assume that $W = 0$ (i.e. no additional source of water except inflow and outflow)

$$J_{in}^c A_c - J_{out}^c A_c = 0, \text{ or}$$

$$Q = J_{in}^c A_c = J_{out}^c A_c = \text{constant}$$

Assumption 3: Once Q is given, we need not worry about water mass balance under such assumptions.

2.2. Some definitions

Mass loading rate (W): Mass $m[M]$ of pollutant entering the system over time period $\Delta t [T]$, $W[MT^{-1}] = m/\Delta t$

Volumetric flow rate (Q): The product of average velocity $U [LT^{-1}]$ entering the system perpendicular to the cross sectional area $A_c [L^2]$, $Q[L^2T^{-1}] = UA_c$.

Mass flux rate (J): Loading rate per unit cross sectional area, $J[MT^{-1}L^{-2}] = W/A_c$.

2.3. Components of pollutant mass balance

The conservation of mass of a substance or a pollutant can be thought of as describing the accumulation of a pollutant within the system in response to what goes in and out. Accumulation = Inflow - Outflow - Reaction - Settling + Loading

2.3.1. Loading

The types of loading that are considered are:

Impulse loading ($W = W_0\delta(t)$): When mass $W_0[M]$ of pollutant enters the system in an instance. Here $\delta(t) [1/T]$ is the dirac delta function, i.e. $\delta(t_0) = \begin{cases} +\infty, & t = t_0 \\ 0, & t \neq t_0 \end{cases}$ such that $\int_{-\infty}^{\infty} f(t)\delta(t_0) dt = f(t_0)$. An accidental spill is an example.

Step loading: When loading rate changes from 0 to a constant value at some point in time. For example a newly established chemical plant starts to spill into a stream flowing close by.

Pulse loading: This is loading type which jumps from 0 to a constant value for a period of time and then jumps back to 0. Note that pulse loading can be obtained as a difference between two step loadings rates. More on this will be discussed later.

Finland's biggest chemical catastrophe in history

Blogpost by Brian Fitzgerald - 9 November, 2012 at 13:54

15 comments

Greenpeace Finland is bearing witness and taking samples at a toxic spill that began on Sunday in the north of the country. The Talvivaara metal mine, owned and operated by Talvivaara Mining Company plc, has been leaking water containing high concentrations of nickel and uranium at a rate of between 5000-6000 cubic metres an hour. It is believed that the leak took place when the mine's waste-water pool was breached on Sunday.



Figure 2.2: Greenpeace and the Talvivaara accident

The Talvivaara accident

A step loading into Finnish surface water bodies in the north of the country in action in Figure 2.2..

2.3.2. Settling and reactions

Settling and reactions are equivalent in the sense

that these two mechanisms take the pollutant or the substance out of the mass balance equation. Setting occurs as a result of certain settling velocity over a certain surface area of the bottom of the system.

Reaction on the other hand can result from certain biological or chemical reactions. Often such reactions are assumed to be a function of the concentration of the pollutants itself. That is, if the concentration of the pollutant within the system is changing only due to the reactions then this means that the rate of change is assumed to be proportional to $f(c)$. Here $f(\cdot)$ is that function. In this course only first order reactions will be considered, which are the cases where $f(c) = c$. This then means that $\frac{dc}{dt} \propto c$. Figure 2.3 is one example of such reaction, of first order phenol concentration decay during an electrolytic treatment.

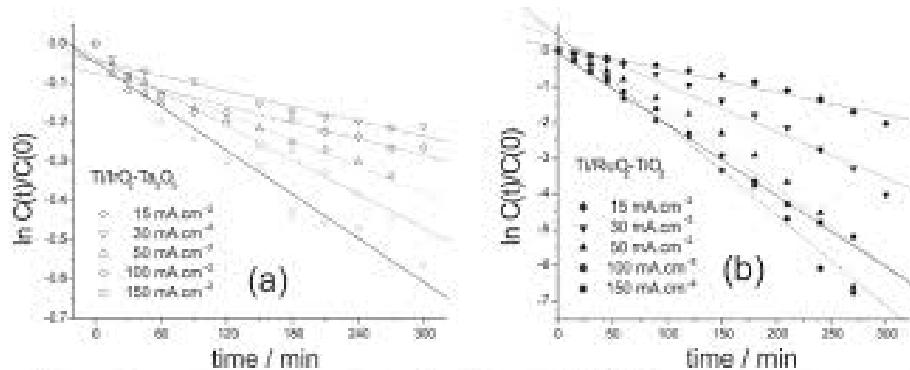


Figure 2.3: Logarithm of normalized concentration decay for the $45\text{SnO}_2/55\text{Ta}_2\text{O}_5$, and for the $70\text{Ta}_2\text{O}_5/30\text{RuO}_2$ electrodes. Solid and empty symbols represent the $70\text{Ta}_2\text{O}_5/30\text{RuO}_2$ and $45\text{SnO}_2/55\text{Ta}_2\text{O}_5$ oxide anodes, respectively.

Figure 2.3: First order decay of phenol. Source:

The constant of proportionality, often represented by $k[1/T]$, is also a measure of time scale at which the pollutants decay, since it is linked to the slope of the tangent to the decay curve at $t=0$ (see Figure 2.4). Thus a slower decay process will have a tangent meeting the x-axis further away from 0.

2.4. System diagnostics

A system can be diagnosed in context of how easy it is to pollute a system and how fast can the system regain back its original state after an accident. Two aspects are studied: susceptibility of a system to pollution and time to recovery after a pollution accident. The former is a steady state concept, i.e. when no change in mass or accumulation of the substance within the system is considered, while the latter is a concept under non-steady state conditions.

2.4.1. Susceptibility to pollution

A completely mixed lake, for example, is considered susceptible if it assimilates (either through reactions, settling or outflow) the pollutants at a slow rate. The assimilation factor depends both on the intrinsic properties of a system such as first order decay coefficient, flow rate, settling velocity as well as the external loading rate of the pollutants. If we assume that water balance is at steady state, the water flows in and out of the system at constant volumetric flow rate Q . Let then the pollutant loading rate be $W = Qc_{in}$.

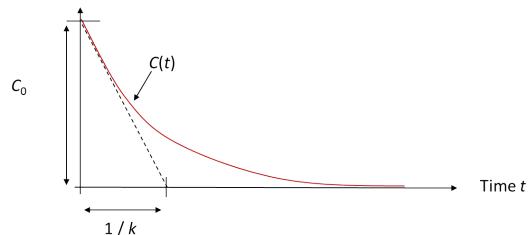


Figure 2.4: The first order decay coefficient is the time scale of the decay process.

From conservation of mass at steady state we know that,

$$V \frac{dc}{dt} = W - Qc - kVc - vA_s c = 0 \quad (2.3)$$

Here, c is the concentration of the pollutant within the system, k is the first order decay rate, V is the system volume, v is the settling velocity, and A_s is the surface area over which the settling occurs.

From this, one can assess the steady state concentration of the system as a function of intrinsic system characteristics and the loading rate. That is,

$$c = \frac{W}{Q + kV + vA_s} = \frac{W}{a}$$

The factor a is called the assimilation factor, which if higher leads to higher rate of assimilation by the lake.

Susceptibility of the Great Lakes, USA:

Smallest of the lakes appear to be most susceptible to pollution due to multiple small lake volume and higher loading rates.

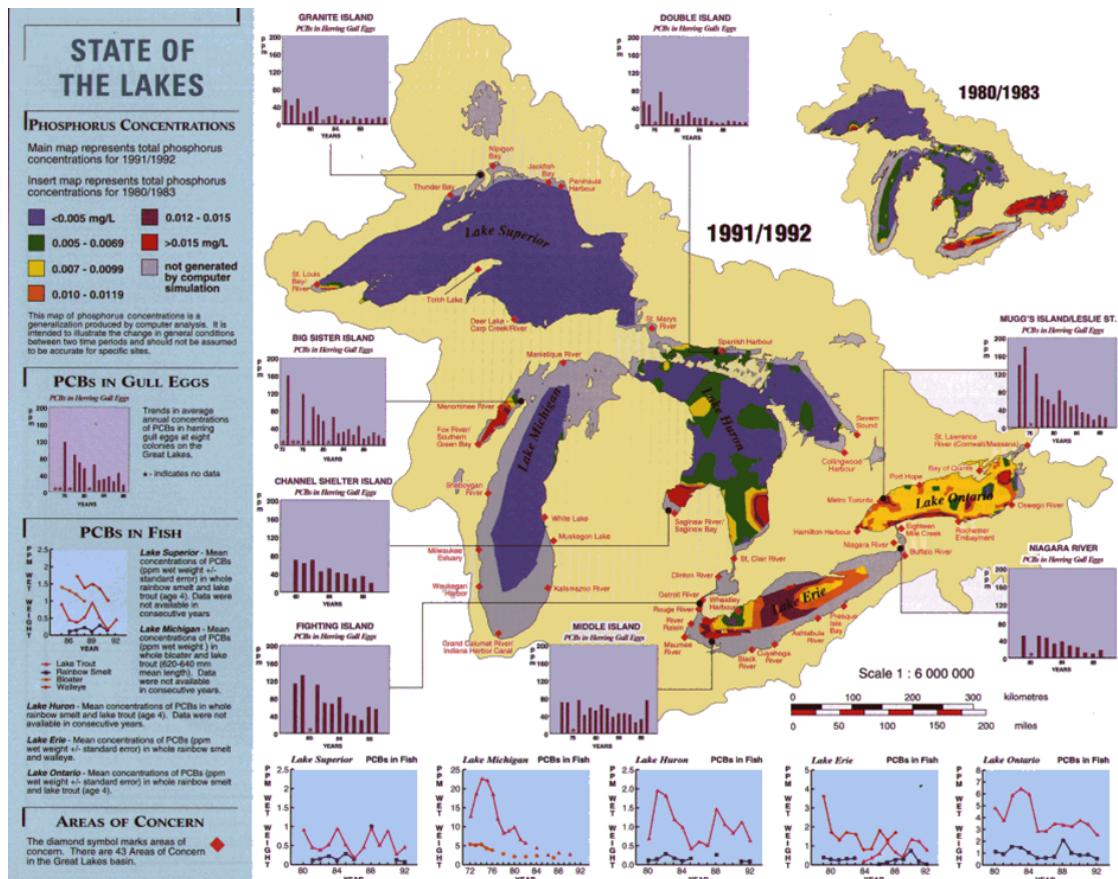


Figure 2.5: The state of the Great Lakes: the smallest of the lakes are the ones most affected. Source:

2.4.2. Residence time and transfer function

Other steady state concepts linked with susceptibility are residence time of pollutants and transfer function of pollutants.

The residence time of a pollutant is the average time that a pollutant spends within a completely mixed system. This is given by,

$$\tau = \frac{V}{Q + kV + vA_s}$$

Meanwhile the transfer function of a system is how the completely mixed system transfers the pollutant concentration in the inflow to what it has in the outflow. From equation 2.3, the steady state function is given by $c = W/a = Qc_{in}$. The transfer function β is the ratio of c_{in} and c , which then can be given as,

$$\beta = \frac{Q + kV + vA_s}{Q}$$

2.4.3. Time to recovery: System dynamics

Resilience of a system is measured by how a system recovers after a pollution accident. This is essentially solving the mass balance differential equation for a certain pollution loading. If the pollutant loading changes, as shown in the figure on the left panel, the system responds in time as shown on the right panel depending on its characteristic. This includes how fast it declines, or how resiliently the system responds to a change.



Figure 2.6: Change in loading rate, e.g. leakage from a chemical plant has been reduced.

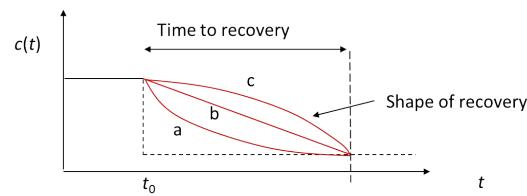


Figure 2.7: The response of the system to the change in the loading rate.

In order to mathematically solve the system, solution to the following differential equation is needed.

$$\frac{dy(x)}{dx} + f(x)y(x) = g(x) \quad (2.4)$$

The solution for the equation above is

$$y(x) = \exp^{-a(x)} \left(\int g(x') \exp^{a(x')} dx' + A \right) \quad (2.5)$$

where $a(x) = \int f(x)dx$ and A is the constant of integration.

For a completely mixed system, the mass balance equation can be simplified into the following form so that a parallel can be drawn with equation 2.4 and the corresponding solution be used.

$$\frac{dc}{dt} + \lambda c = \frac{W(t)}{V} \quad (2.6)$$

Here $\lambda = \frac{Q}{V} + k + \frac{vA_s}{V}$. The following correspondence can then be plugged in equation 2.5 to obtain the solution of how concentration changes over time.

Equation 2.6	Equation 2.4
$c(t)$	$y(x)$
λ	$f(x)$
$\frac{W(t)}{V}$	$g(x)$
λt	$a(x)$

How would then a system recover from an instantaneous loading at time $t = t_0$? - Note that $W(t) = W_0\delta(t)$ in case of instantaneous loading.

Substituting variable definitions in Equation 2.5, the response function of a completely mixed system to an instantaneous loading at time t greater than t_0 , is given by,

$$\begin{aligned} c(t) &= \exp^{-\lambda t} \left(\int \frac{W_0\delta(t_0)}{V} \exp^{\lambda t'} dt' + A \right) \\ &= \frac{W_0}{V} \exp^{-\lambda(t-t_0)} + A \exp^{-\lambda t} \end{aligned} \quad (2.7)$$

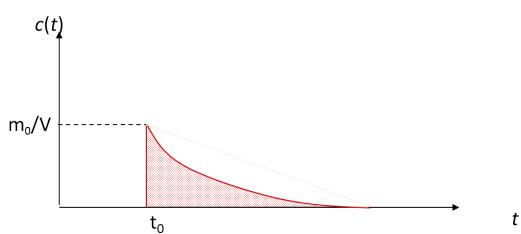


Figure 2.8: System response to an instantaneous load, assuming that the background concentration is 0. Here W_0 is replaced by m_0 .

If the background concentration or the concentration before the onset of instantaneous load is given by c_0 , then we can solve for A by noting that as $t \rightarrow \infty$, $c(t) \rightarrow c_0$. This means that $A = c_0 \exp^{-\lambda t}$. Note that for $t < t_0$, $c(t) = c_0$.

Thus,

$$c(t) = \begin{cases} c_0, & t < t_0 \\ \frac{W_0}{V} \exp^{-\lambda(t-t_0)} + c_0, & t \geq t_0 \end{cases}$$

See also Figure 2.8. Similarly the solution for the case when a system is hit by a step load can be obtained. Following is the solution for a system response to a step load of type,

$$W(t) = \begin{cases} 0, & t < t_0 \\ W_{\text{cst}}, & t \geq t_0 \end{cases}$$

$$\begin{aligned} c(t) &= \exp^{-\lambda t} \left(\int \frac{W_{\text{cst}}}{V} \exp^{\lambda t'} dt' + A \right) \\ &= \frac{W_{\text{cst}}}{\lambda V} \exp^{-\lambda(t-t_0)} + A \exp^{-\lambda t} \end{aligned} \quad (2.8)$$

Since for $t \leq t_0$, $c(t) = 0$, and $t \rightarrow \infty$, $c(t)$ is a non-zero constant, we need $A = A_0 \exp^{-\lambda t}$ where A_0 is a constant. But then for $t = t_0$, $c(t_0) = 0$, which means that $A_0 = \frac{W_{\text{cst}}}{\lambda V}$. Plugging this back in Equation 2.8, we obtain how a surface water body reacts to a constant loading.

$$c(t) = \begin{cases} 0, & t < t_0 \\ \frac{W_0}{\lambda V} (1 - \exp^{-\lambda(t-t_0)}), & t \geq t_0 \end{cases}$$

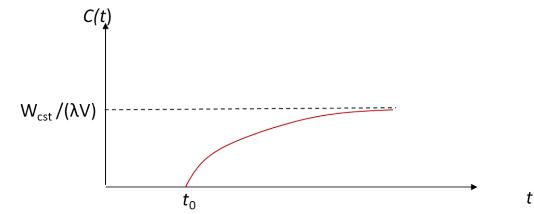


Figure 2.9: System response to a step load, assuming that the background concentration is 0.

2.5. Principle of superposition

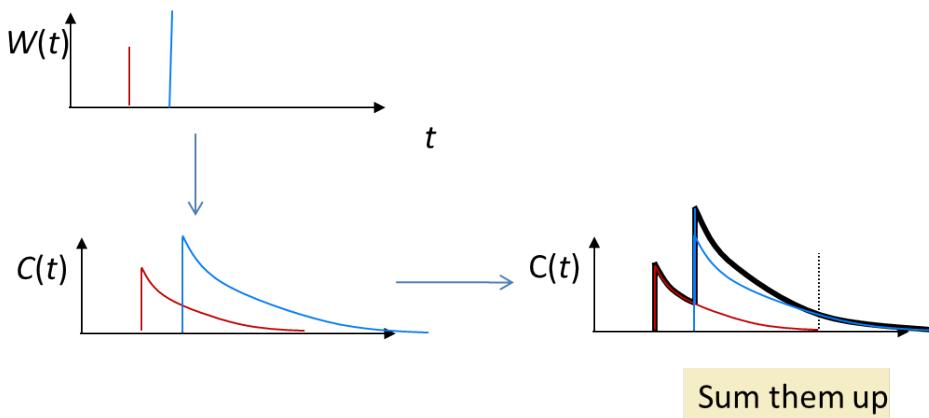


Figure 2.10: Principle of superposition: If the system is linear then system response to 2 or more loadings is the sum of individual responses to the loadings.

The mass balance of pollutants in Equation 2.6 is a linear differential equation. This is because λ in the equation is not a function of c . This means that if $c_1(t)$ is the solution of $\frac{dc}{dt} + \lambda c = \frac{W_1(t)}{V}$ and $c_2(t)$ is the solution of $\frac{dc}{dt} + \lambda c = \frac{W_2(t)}{V}$ then $c_1(t) + c_2(t)$ is the solution of $\frac{dc}{dt} + \lambda c = \frac{W_1(t) + W_2(t)}{V}$. This is because $c_1(t) + c_2(t)$ satisfies $\frac{dc}{dt} + \lambda c = \frac{W_1(t) + W_2(t)}{V}$, which can be tested by plugging $c_1(t) + c_2(t)$ into $\frac{dc}{dt} + \lambda c \Rightarrow \frac{dc_1(t)}{dt} + \lambda c_1(t) + \frac{dc_2(t)}{dt} + \lambda c_2(t) = \frac{W_1(t) + W_2(t)}{V}$.

The statement of the principle of superposition is as follows: if the system response can be represented by a linear differential equation then the response of the system to 2 or more loadings can be obtained from the sum of individual responses to the loadings.

One important aspect of this principle is convolution. If one notes the solution to the differential equation, one can see that $\int \frac{W(t)}{V} \exp^{\lambda(t'-t)} dt'$ is the convolution operation that is linear in $W(t)$ and determines the response of the system loading $W(t)$. Here if $W(t)$ is replaced by $W_1(t) + W_2(t)$ then the total response becomes the sum of two individual responses, i.e.

$$\int \frac{W_1(t) + W_2(t)}{V} \exp^{\lambda(t-t')} dt' = \int \frac{W_1(t)}{V} \exp^{\lambda(t-t')} dt' + \int \frac{W_2(t)}{V} \exp^{\lambda(t-t')} dt'$$

3

Incompletely mixed systems

This chapter deals with incompletely mixed systems. Lakes and rivers that are not completely mixed with, e.g. salt, have varying concentration of such substances within their system boundaries. The mass balances of water and the substances are needed to be solved. Note that since concentrations change in both space and time, mass balance equations for the substances involved are specified both in space and time.

3.1. Topics to be covered

1. Diffusion and diffusion equation
2. Advection and advection equation
 - 1d plug flow model
 - Similarity between plug flow model and feedforward cascade model (from completely mixed systems)
3. Systems containing diffusion, advection and decay simultaneously
4. Steady state solution for Advective Dispersive Equation (ADE) with decay

3.2. Diffusion only system

3.2.1. A conceptual model for diffusion

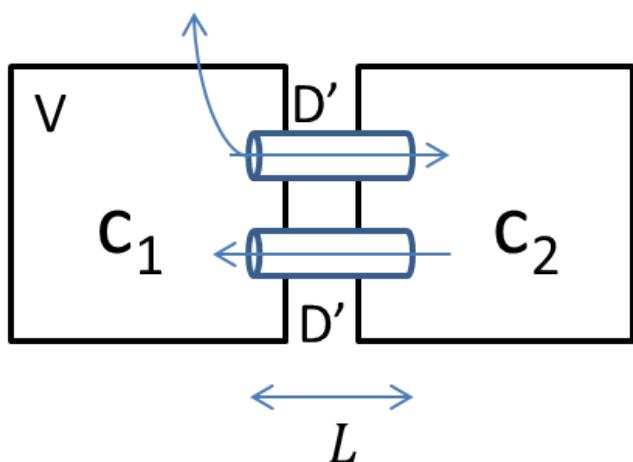


Figure 3.1: A conceptual model for diffusion

Diffusion is often conceptualized as resulting from a giant mixer, that moves around water with different concentrations of a substance, e.g. salt. The following provides a more intuitive explanation of diffusion.

Consider the Figure 3.1, which visualizes the same. One would expect that mass flux of substances flows from high concentration levels to low concentration levels. This is also called the Fick's first law, which states that mass flux rate of a substance is proportional to the negative of the concentration gradient, $J \propto -\frac{\partial c(x,t)}{\partial x}$. For the discretized case as shown in Figure 3.1, $J = D \frac{c_2 - c_1}{L}$, where D is the constant of proportionality called the diffusion coefficient. Following the law, the conservation of mass for the left reservoir can be given by (assuming positive x-axis is from the left to the right),

$$V \frac{dc_1(t)}{dt} = -\left(-DA_c \frac{c_2 - c_1}{L} \right) \quad (3.1)$$

Here, the area of cross section across which the diffusion happens appears in order to convert mass flux rate, which mass rate per unit area, to mass rate for it to be consistent with the left hand side of the equation.

Now lets consider another perception. The two reservoirs taken together form an incompletely mixed system since the concentration varies in space. We can think of diffusion as a mechanism that mixes the water from left to right and then right to left reservoir with volumetric flow rate D' . The conservation of mass for the left reservoir can again be calculated as,

$$V \frac{dc_1(t)}{dt} = D' c_2 - D' c_1 \quad (3.2)$$

The equation 3.2 allows us to interpret the diffusion coefficient. By matching the right hand sides of equations 3.1 and 3.1, we note that $D' = \frac{DA_c}{L}$, or,

$$D = \frac{D'L}{A_c} \quad (3.3)$$

That is, diffusion coefficient is scale sensitive. It scale with the length of mixing and inversely with the area of cross section across which it mixes. Diffusion (dispersion, convection, conduction) is often referred to by different names, depending on the context. The figure below (Figure 3.2) demonstrates its scale sensitivity in those different contexts.

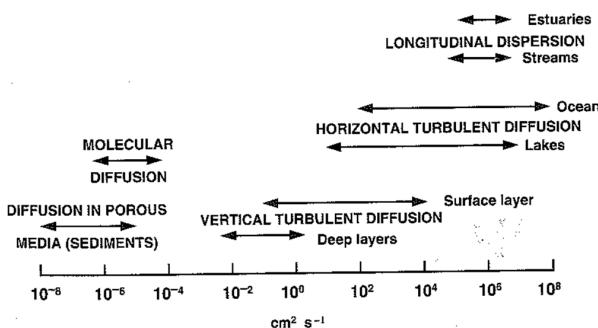


FIGURE 8.10
Typical ranges of the diffusion coefficient in natural waters and sediments.

Figure 3.2: Scale dependency of the dispersion coefficient: Source: The Chapra book

Given that we are now dealing with incompletely mixed systems where in the concentration of substances can vary in both space and time, we adapt the definitions of different types of loading as in the following:

Instantaneous point spill: a spill (or loading) at one instance in time and one point in space

Continuous point spill: a spill continuous in time but at one point in space

Instantaneous nonpoint/distributed spill: a spill instantaneous in time but distributed in space

Continuous nonpoint/distributed spill: a spill that does not stop anytime and is distributed in space

Having conceptualized the dispersion coefficient, we now derive the mathematical equation for conservation of mass for incompletely mixed systems when only dispersion is present.

3.2.2. Fundamental equation

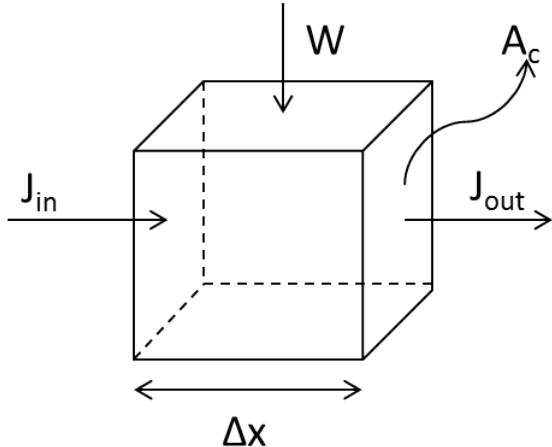


Figure 3.3: A differential element within which conservation of mass is applied.

The mass flux in case of diffusive systems is given by Fick's first law, i.e. $J = -D \frac{\partial c}{\partial x}$. Also, since concentration now changes in both space and time, i.e. $c(x, t)$, we start using partial derivatives. The loading rate is now also a function of both space and time, i.e. $W(x, t)$, which we assume scales linearly with x . This means that we are only seeking 'partial' changes of concentration with space or with time. The mass balance corresponding to Figure 3.3 can be given as,

$$V \frac{\partial c}{\partial t} = J_{in} A_c - J_{out} A_c + W \quad (3.4)$$

From Fick's law we obtain $J_{in} = -D \frac{\partial c}{\partial x}$. And since the element that we are considering in Figure 3.3 is a differential element, we expect J_{out} to be not too different from J_{in} . Thus we can approximate J_{out} in terms of J_{in} , for which we use Taylor series expansion. By Taylor series expansion, we get

$$\begin{aligned} J_{out} &= J_{in} + \frac{\partial J_{in}}{\partial x} \Delta x + \mathcal{O}(\Delta x^2) \\ &= J_{in} - D \frac{\partial^2 c(x)}{\partial x^2} \Delta x + \mathcal{O}(\Delta x^2) \end{aligned} \quad (3.5)$$

Here, $\mathcal{O}(\Delta x^2)$, means that the terms expands or contracts at the same rate as Δx^2 . Plugging Equation 3.5 in Equation 3.4, we obtain the mass balance equation for diffusive systems as,

$$\begin{aligned} A_c \Delta x \frac{\partial c}{\partial t} &= D \frac{\partial^2 c(x)}{\partial x^2} \Delta x A_c - \mathcal{O}(\Delta x^2) A_c + A_c \Delta x W \\ \Rightarrow \frac{\partial c}{\partial t} &= D \frac{\partial^2 c(x)}{\partial x^2} - \frac{\mathcal{O}(\Delta x^2)}{\Delta x} + W \end{aligned} \quad (3.6)$$

As $\Delta x \rightarrow 0$, which means that the element becomes really small in the limit, the mass balance equation becomes,

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c(x)}{\partial x^2} + W$$

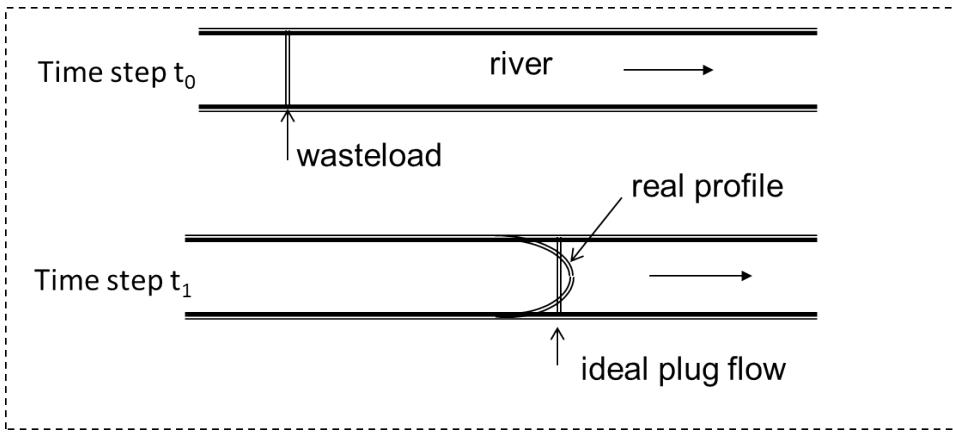


Figure 3.4: Plug flow: Advection only system.

If one also witnesses first order decay of the substance, i.e. $-kc$, then the equation becomes,

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c(x)}{\partial x^2} - kc + W \quad (3.7)$$

3.2.3. Steady state solution

Note that steady state solution means that the concentration does not change in time. That means the loading rate must remain constant in time, i.e. continuous. Steady state solution for arbitrary loading can be obtained as solution to so called second order inhomogeneous differential equation given in equation 3.7

Following is the steady state solution for continuous load at one point in space, assuming that the concentration at the point where loading happens is c_0 , is

$$c(x) = c_0 \exp^{-\sqrt{\frac{k}{D}}|x|}$$

3.3. Advection only system

Advection only systems are easier to understand. Here the pollutant flows along with the flow velocity (see Figure 3.4).

3.3.1. Fundamental equation

If the flow velocity is given by U , mass flux rate can be given by $J = Uc$. Similar to the derivation of the fundamental equation for diffusion only system, we can obtain the mass balance equation for advection only system.

If $J_{in} = Uc$, then $J_{out} \approx Uc + U \frac{\partial c}{\partial x} \Delta x$ and the advection only equation in the limit becomes

$$\frac{\partial c}{\partial t} = -U \frac{\partial c(x)}{\partial x} - kc + W \quad (3.8)$$

3.3.2. Steady state solution

Steady state solution with point source pollution is given by $c(x) = c_0 \exp^{-\frac{k}{U}x}$, where c_0 is the concentration of the pollutant at $x = 0$. Note that since the solution is at steady state, this requires that the loading is continuous in time at $x = 0$ resulting in concentration c_0 at $x = 0$. If the point loading occurs at $x = x_0$, then the solution can be changed to,

$$c(x) = c_0 \exp^{-\frac{k}{U}(x-x_0)} \quad (3.9)$$

Note that the case where there is no decay, then $c(x) = c_0$ for all x because the pollutant will be carried continuously carried along the stream at constant velocity U .

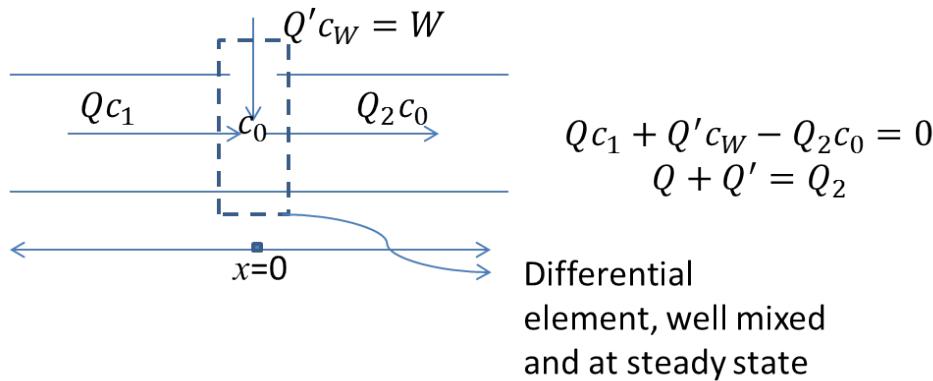


Figure 3.5: Why $c_0 = W/Q$ under no diffusion when the point (continuous) loading at $x = 0$ is W .

In case when one is given a certain amount of continuous point loading, $W\delta x_0$, instead of concentration, c_0 at x_0 , one can obtain c_0 as $\frac{W}{Q}$ for *Advection only* system as follows.

Consider an infinitesimally small element around $x_0 = 0$ in Figure 3.5. Water flows in with volumetric flow rate of Q and with concentration of pollutant at c_1 . The pollutant loading occurs at $x = 0$ riding on relatively low volumetric flow rate Q' at concentration c_W such that $W = Q'c_W$. This loading mixes with the incoming concentration to yield concentration c_0 at $x = 0$. What exactly is the c_0 can be obtained by applying conservation of mass both for pollutants and water at steady state.

$$\text{Pollutant conservation of mass: } Qc_1 + Q'c_W - Q_2c_0 = 0$$

$$\text{Water conservation of mass: } Q + Q' = Q_2$$

The above gives us $c_0 = \frac{Qc_1 + W}{Q + Q'}$. If Q' is relatively small, then the volume flowing out is almost equal to the amount flowing in from the left, i.e. $Q_2 \approx Q$. Thus, if incoming concentration is 0 and the pollutant enters the system only at $x = 0$, we obtain $c_0 = \frac{W}{Q}$. Therefore, the solution in Equation ?? may as well be given by,

$$c(x) = \frac{W}{Q} \exp^{-\frac{k}{U}(x-x_0)}$$

3.3.3. Interconnected completely mixed systems

An incompletely mixed system can be represented by serially connected completely mixed systems. This demonstrates that a more complex incompletely mixed system can be represented by simpler completely mixed systems. That is, a more complex system representation can be formulated in the form of simpler completely mixed systems.

To do so, let's first understand how water that is flowing in with flow rate Q and bringing pollutant with it at concentration c_{in} would carry the pollutant through a series of interconnected completely mixed reservoirs. All these calculations will be done at steady state.

Applying conservation of mass in the first reservoir, we obtain $Qc_{in} - Qc_1 - kc_1V = 0$. This means that $c_1 = \frac{Qc_{in}}{Q+kV}$. For any i^{th} , we obtain $c_i = \frac{Qc_{i-1}}{Q+kV} = \left(\frac{Q}{Q+kV}\right)^2 c_{i-2} = \dots = \left(\frac{Q}{Q+kV}\right)^i c_{in}$.

Now we can explore what is the connection between the equation above and the plug flow Equation 3.9. We would expect the descriptions to converge as $\Delta x \rightarrow 0$ in Figure 3.6 since that is how Equation 3.9 was obtained using Taylor series approximation. Since $V = A_c \Delta x$ and $i = \frac{x}{\Delta x}$,

$$\begin{aligned} \lim_{\Delta x \rightarrow 0} c_i &= \lim_{\Delta x \rightarrow 0} \left(\frac{Q}{Q+kA_c \Delta x}\right)^{\frac{x}{\Delta x}} \\ &= \lim_{\Delta x \rightarrow 0} \left(1 + \frac{k}{U} \Delta x\right)^{\frac{-x}{\Delta x}} \end{aligned} \tag{3.10}$$

Given that $\exp^x = \lim_{n \rightarrow \infty} \left(1 + \frac{x}{n}\right)^n$, we see that the solution of how interconnected completely mixed system converges to the solution given in Equation 3.9.

$$\lim_{\frac{-x}{\Delta x} \rightarrow \infty} c_i = \lim_{\frac{-x}{\Delta x} \rightarrow \infty} \left(1 - \frac{kx/U}{\frac{-x}{\Delta x}}\right)^{\frac{-x}{\Delta x}} = c_{in} \exp^{-\frac{k}{U}(x-x_0)} \quad (3.11)$$

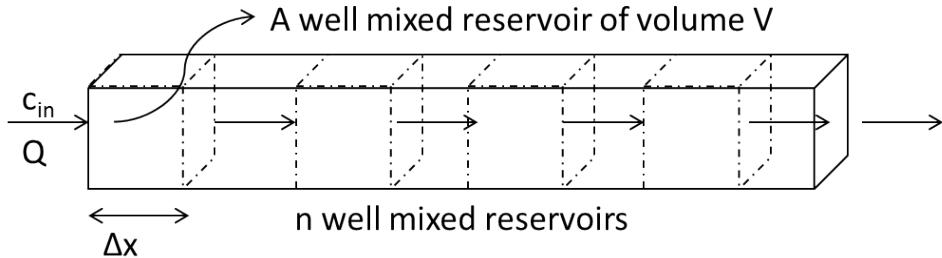


Figure 3.6: Plug flow cascading through a series of completely mixed reservoirs

3.4. Mixed Flow: Advection, dispersion with decay (ADE)

The mixed flow is when both advection and diffusion (dispersion) occur.

3.4.1. Fundamental equation

The equation for advection, dispersion with decay transport of pollutants or substances can be obtained in a similar manner as diffusion only or dispersion only equations (i.e. using Taylor series approximation for a infinitesimally small element as shown in Figure 3.3. The key to obtaining the equation is to note that $J_{in} = Uc_{in} - D\frac{\partial c(x)}{\partial x}$ for mixed flow. Following the same steps as given in Equations 3.5, we obtain the following equation,

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c(x)}{\partial x^2} - U\frac{\partial c(x)}{\partial x} - kc + W \quad (3.12)$$

3.4.2. Steady state solution

How an ADE system behaves in the long run when the system is polluted by a continuous point source at rate $W_0\delta(x - x_0)$? The following, which is the solution to Equation for $\frac{\partial c}{\partial t} = 0$ and $W = W_0\delta(x - x_0)$.

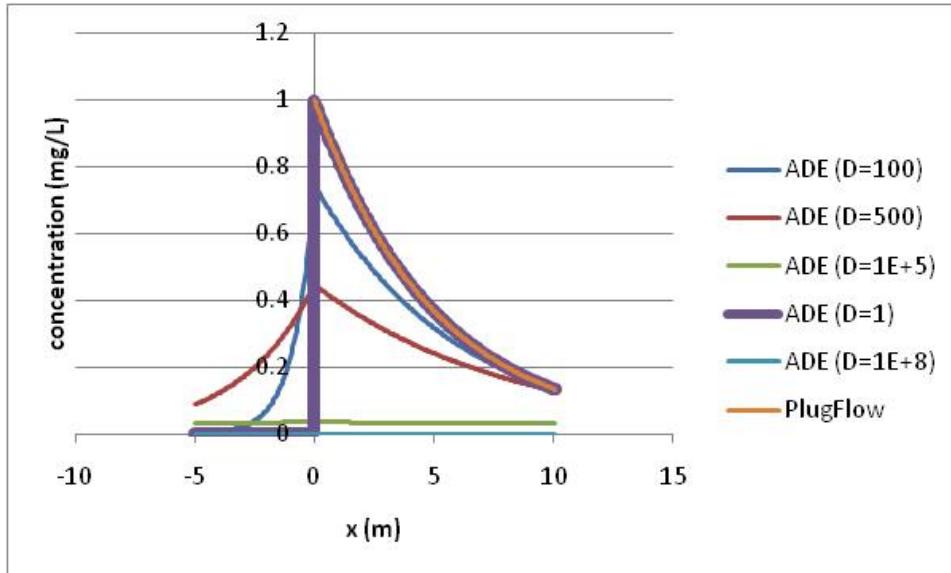


Figure 3.7: Upper and lower limits of Mixed flow model at steady state

$$\begin{aligned}
 c &= \frac{W}{Q\sqrt{1+4\eta}} \exp^{\frac{U}{2D}(1+\sqrt{1+4\eta})} \quad x < 0 \\
 c &= \frac{W}{Q\sqrt{1+4\eta}} \exp^{\frac{U}{2D}(1-\sqrt{1+4\eta})} \quad x \geq 0
 \end{aligned}
 \tag{3.13}$$

where, $\eta = \frac{kD}{U^2}$.

The Figure 3.7 shows that the upper limit of the solution to ADE with respect to D is plug flow while the lower limit is a completely mixed system. This shows that both diffusion only system and advection only systems are 'mixed' together in ADE. This also smells of principle of superposition.

Figure 3.7 shows ADE solutions for various values of D (sq m./hr) as well as plug flow equation for $\frac{W}{Q}=1\text{mg/L}$, $k=20/\text{hr}$, $U=100\text{ m/hr}$ and $A_c=10\text{ sq m}$. Note that for $D=1\text{ sq m hr}$, ADE steady state solution is the same as the solution of plug flow model for continuous point loading at $x=0$, while for large D , it spreads out the concentration.

3.5. Non-steady state solutions

The non-steady state solutions mean that the loading rate is not necessarily continuous in time but can change. The solutions that are presented below are for instantaneous point load and since the equation is linear in concentration, this means that solutions of instantaneous point loads of different magnitudes can be superimposed to obtain a final solution.

3.5.1. Advection only system

The solution is similar to the one at steady state, except that one has to 'run' with injected plug to follow how the corresponding concentration changes in time. If the instantaneous point loading is such that $c(t=0, x=0) = \frac{W\delta(t,x)}{Q} = c_0$, then solution to the Advection only equation,

$$\frac{\partial c}{\partial t} = -U \frac{\partial c}{\partial x} + W$$

can be given by,

$$\begin{aligned}
 c(t, x) &= 0 \quad x \neq Ut \\
 c(t, x) &= c_0 \exp^{-\frac{kx}{U}} \quad x \neq Ut
 \end{aligned}
 \tag{3.14}$$

Figure 3.8 illustrates the concept.

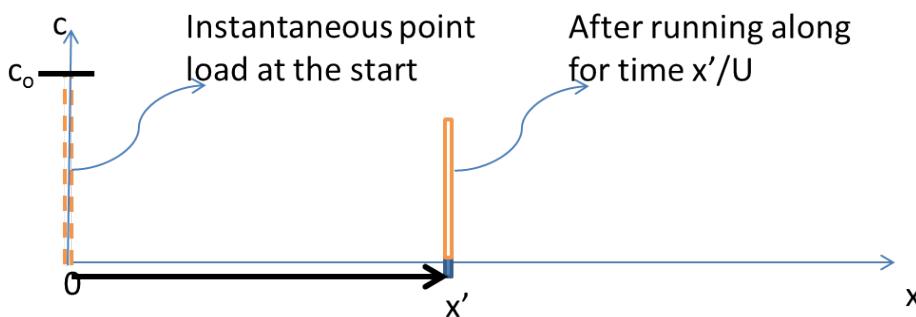


Figure 3.8: Advection only with decay in time

3.5.2. Diffusion only system

Imagine a droplet of ink dropped (see Figure 3.9). One would imagine that drop of ink to gradually diffuse out and expand in size with the concentration being always the highest at the location where the ink was dropped, gradually waning out as one moves away from that point.

This exemplify how diffusion occurs over time, i.e. what is the solution of the following differential equation for instantaneous point load ($W = W_0\delta(x, t)$),

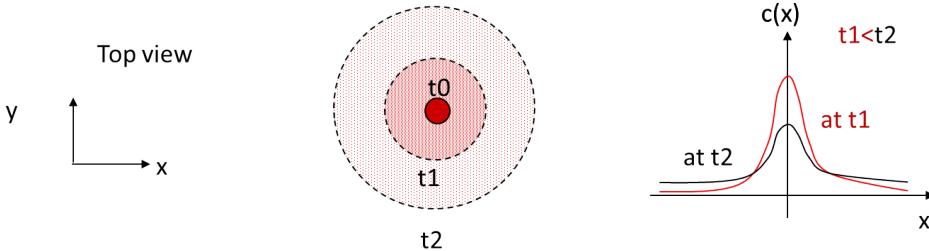


Figure 3.9: Diffusion only with decay in time

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} + W$$

The solution is given by,

$$c(t, x) = \frac{W_0}{A_c \sqrt{\pi D t}} \exp^{-\frac{x^2}{4Dt}} \quad (3.15)$$

The intuition behind the solution is as follows. Imagine a drunk crowd (see Figure ??), say of unit mass, coming out of a pub after closing hours. A few of them take left and other take right. So at each time step Δt , an individual within the crowd takes 1 step of size Δx , either to the left or to the right. The former group further disperses, some taking left and others right. Same goes for the second group. Over time, any individual may cross another many times while, overall, the crowd disperses in space just as the drop of ink disperses over time in Figure 3.9.

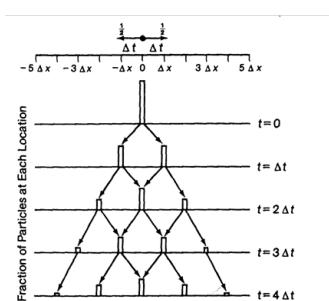
If any individual being a drunk has equal probability moving to the left or the right, then one can estimate the chance of finding a drunk individual at n_t time steps at n_x steps away from the pub (in the positive x direction). This is given by,

$$P(n_x, n_t) = (1/2)^{n_t} \frac{n_t}{(\frac{n_t+n_x}{2})! (\frac{n_t-n_x}{2})!}$$

As we reduce time and distance steps to infinitesimally small, i.e. $\Delta t \rightarrow 0, \Delta x \rightarrow 0$, we obtain the solution given in Equation 3.15, that is,

$$\lim_{\Delta t \rightarrow 0, \Delta x \rightarrow 0} P(n_x, n_t) = \frac{W_0}{A_c \sqrt{\pi D t}} \exp^{-\frac{x^2}{4Dt}} \quad (3.16)$$

with $t = n_t \Delta t$, $x = n_x \Delta x$ and $D = \frac{\Delta x^2}{2\Delta t}$.



Source: Surface Water Quality Modeling by Steven Chapra

Graphic representation of a random walk. At time $t = 0$, all particles are grouped at the origin ($x = 0$). During each time step Δt , half the particles at each location move left and half move right. The result is that over time the particles spread out in a bell-shaped pattern.

Figure 3.10: Drunk walk and how concentration varies in dispersion only systems

3.5.3. Advection with Dispersion system with decay

The same intuition behind how a dispersion only system behaves over time can be extended to mixed systems with advection. This can be done by imagining that in addition to random walk to the left and the right, all individuals also drift to the right by amount $U\Delta t$. The positions of all the individuals have to be corrected by $\Delta x = U\Delta t$ for the above solution to dispersion only system to be applicable. This means that the following solution holds for Advection and dispersion system,

$$c(t, x) = \frac{W_0}{A_c \sqrt{\pi D t}} \exp^{-\frac{(x-Ut)^2}{4Dt}} \quad (3.17)$$

Noting that if there is first order decay process that eats up the pollutant over time, the same equation can be extended to obtain transient solution for ADE with decay as,

$$\begin{aligned} c(t, x) &= \frac{W_0}{A_c \sqrt{\pi D t}} \exp^{-\frac{(x-Ut)^2}{4Dt}} \exp^{-kt} \\ &= \frac{W_0}{A_c \sqrt{\pi D t}} \exp^{-\frac{(x-Ut)^2}{4Dt} - kt} \end{aligned} \quad (3.18)$$

The Equation 3.18 is the very basic version of Rhine Alarm Model (v1.0), also called Taylor model.

Another form of the same equation can be obtained by substituting $Q = UA_c$ in the denominator and moving the terms around in the exponent.

$$= \frac{W_0}{Q \sqrt{\pi \frac{Dt}{U^2}}} \exp^{-\frac{(t-\frac{x}{U})^2}{4Dt/U^2} - kt}$$

Figure 3.11 illustrates the solution, the observer has to run with velocity U to witness a Gaussian pollutant cloud gradually dispersing (becoming flatter over time) and decaying (pollutant mass disappearing due to the decay).

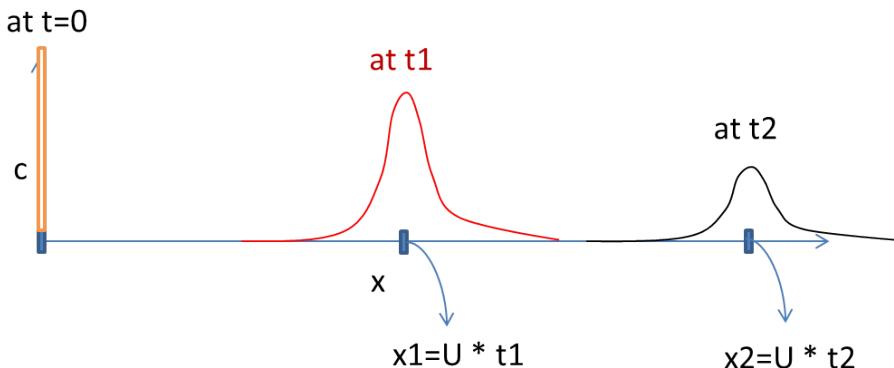


Figure 3.11: Illustration of how pollution wave travels in space and time when advective, dispersion and decay are active

One may therefore end up thinking that one always sees a Gaussian, i.e. symmetric bell shaped, pollutant cloud. This however only occurs when one is running along with the pollution cloud. What happens when one is stationary, waiting at one location, for the pollution to arrive? This is something similar to a town downstream of river Rhine, for example, waiting for a pollution 'wave' to arrive after an industrial accident somewhere in Germany!

One key aspect to note when seeing a pollution wave passing by is that while the wave is passing through a town, it is also dispersing. Thus, the trailing end keeps getting elongated as one waits for the entire wave to pass by - this is the dispersive effect relative to advection. As a result, one observes an asymmetric pollution wave at one location (see Figure 3.12).

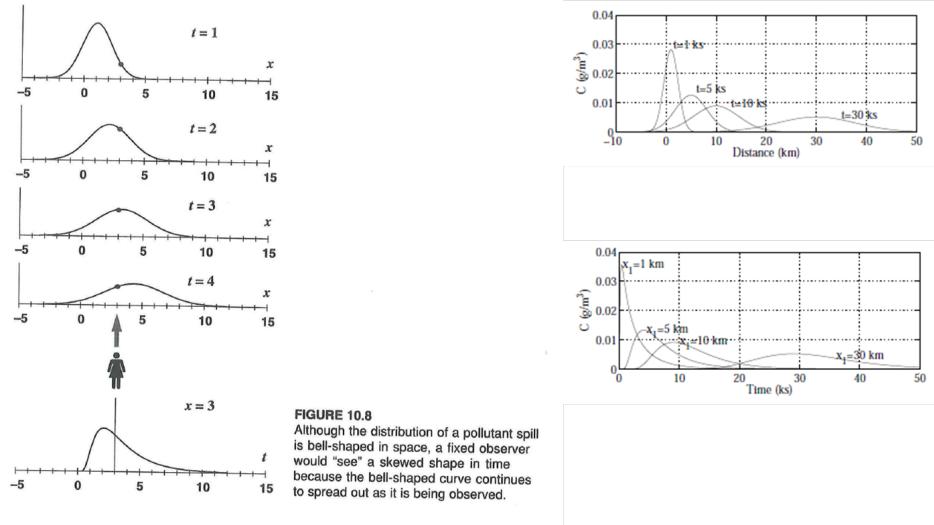


Figure 3.12: One observes an asymmetric pollution wave at a location.

Second key aspect is that the dispersive effect relative to advection is stronger earlier in time. This is also when one is closer to the source of pollution (or the loading point). The dispersive effect disappears far off from the source because by then dispersion has already smoothed out contrasts in concentration of the pollutant due to mixing, especially at the edges of the cloud. The concentration gradient in space at any time far from the pollution accident becomes very small, leading to significantly small diffusion fluxes (which by Fick's law $\propto \frac{\partial c}{\partial x}$). Therefore at far off location, the pollution cloud travels past a point as if it were a Gaussian 'plug' (as if there is no dispersion and the pollutant plug is of Gaussian shape) and the pollution flow is only advective with decay.

4

Rhine Alarm Model

The Taylor model described in Chapter 3 has been developed for idealized conditions. This means that it can provide a first order assessment of reality on the ground. The cross sectional geometry has been assumed not to change with distance, with a rectangular cross sectional area. Also, the flow through any reach is assumed to have been unperturbed by stagnant zones. These stagnant zones not only reduce the effective cross sectional area through which the water flows, but also stagnate pollutant flow. These zones can therefore also act as transient storage for pollutants (Figure 4.1).

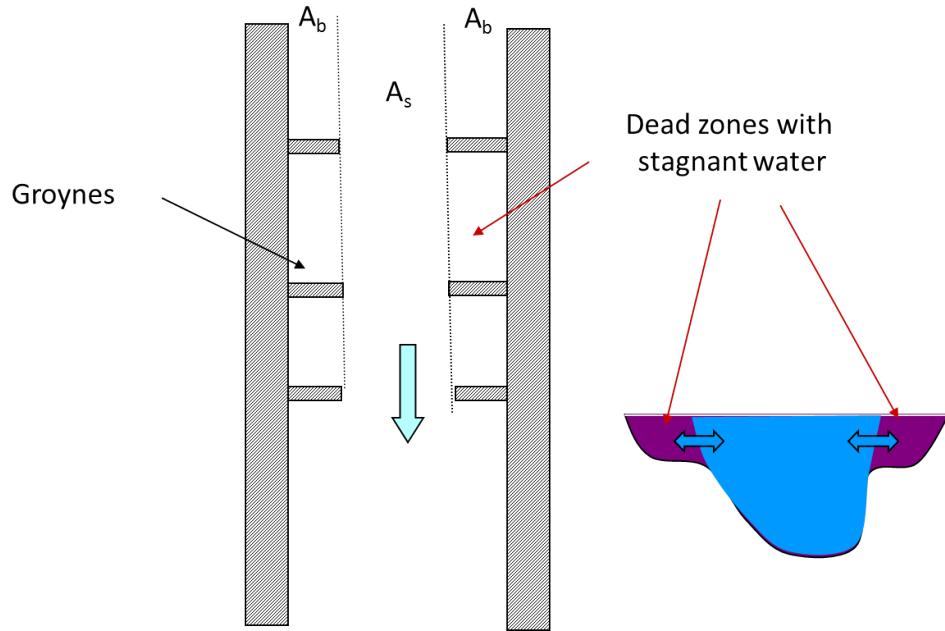


Figure 4.1: Stagnant zone and a need for a more realistic conceptualization of Advection and Dispersion to model transport phenomenon in surface water bodies.

4.1. Fundamental Equation

In order to incorporate the asymmetries that are possibly introduced due to existence of groynes, a factor is multiplied to the Taylor model. The following provides the formulation behind this adapted version of the Taylor model.

$$c(x, t) = \frac{W}{Q\sqrt{4\pi D_0 t/c^2}} \exp^{-\frac{(t-x/c)^2}{4D_0 t/c^2}} \left[1 + \frac{G_t}{6} H_3 \left(\frac{t-x/c}{\sqrt{2D_0 t/c^2}} \right) \right] \quad (4.1)$$

Two main differences between Equation 4.1 and the Taylor Model discussed in the previous chapter can be noted. First is the use of c instead of U and the second is the multiplicative factor, which essentially adapts the Taylor model to real world applications. Following provides the description of various variables.

The variable c is the transport velocity that accommodates the reduction of effective cross section area. It is given by $c = \frac{U}{1+\beta_{\text{local}}}$, where $\beta_{\text{local}} = \frac{A_b}{A_s}$ is the ratio of reduced area to the area closed by groynes (see Figure 4.1).

D_0 is the dispersion coefficient which is partly calibrated based on the predictive equation, such as $D_0 = \frac{\alpha U^2 B_s^2}{au_*}$, can be used. Here α is the parameter to be calibrated, a is the average water depth, u_* is the shear velocity given by $\frac{U\sqrt{g}}{25(5a)^{1/6}}$ and B_s is the width of the main stream.

Yet another parameter that needs to be calibrated is in the multiplicative factor. It is called the skewness parameter G_t , which is supposed to be $\frac{g_t}{\sigma_t^3}$. Here g_t is the 3rd moment of a skewed wave at time t and σ_t is the variance of the wave.

Finally, $H_3(\bullet)$ is a 3rd Hermite polynomial $H_3(z) = z^3 - 3z$.

4.2. Calibrating the Rhine Alarm Model

Thus there are 3 'parameters' that need to be calibrated. One may calibrate α and β_{local} and then estimate the skewness factor G_t based on the observed wave. Calibration is done by simulating a pollution accident. That is, a tracer solution with certain concentration c_0 is spilled at x_0 and concentration wave is measured at some location downstream, say $x > x_0$. The parameters are then 'tweaked' to match predicted concentration profiles with the observed.

Figure 4.2 is one example of this.

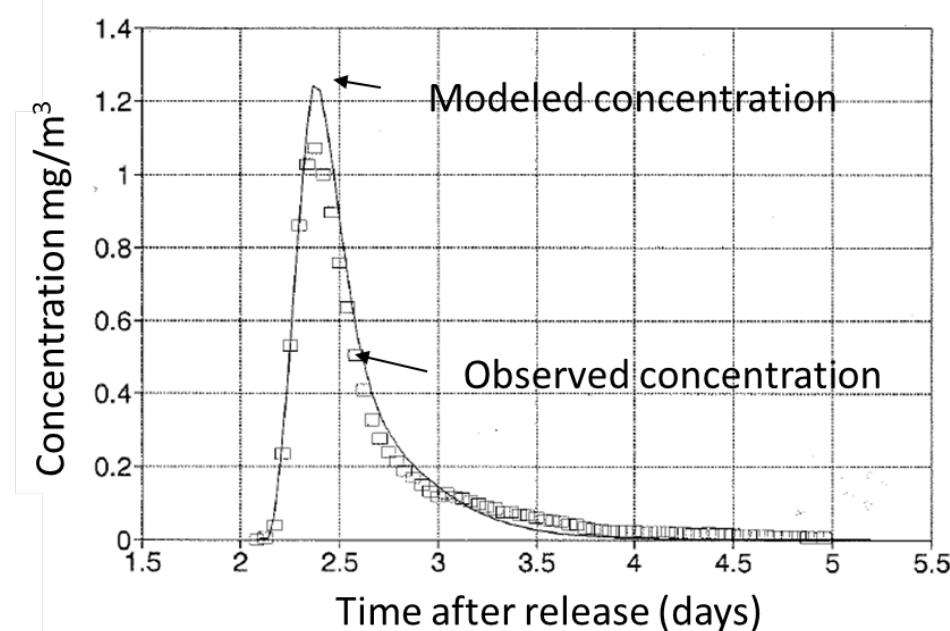


Figure 4.2: The parameters α and β_{local} are tweaked so that the concentration profile predicted by the model at Maximiliansau matches that which is measured.

Since the dispersion coefficient is scale dependent (and also that is being calibrated), one expects it to increase in magnitude as one moves downstream. Figure 4.3 below shows how the dispersion coefficient which has been calibrated varies as one goes downstream. This is possibly due to larger mixing lengths per unit cross sectional area as well as larger volumes of water being mixed.

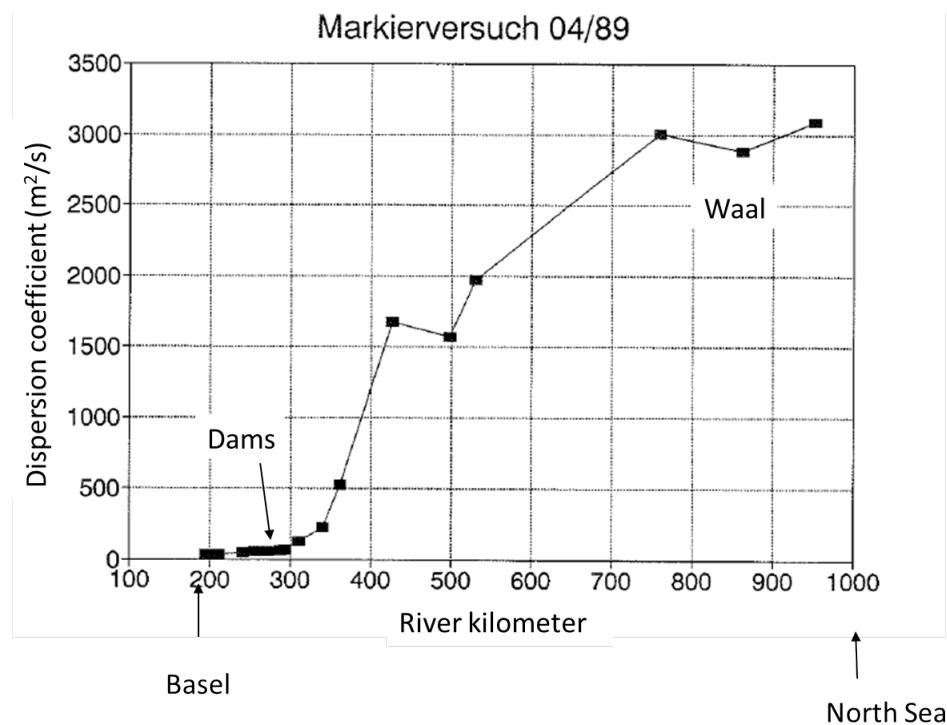


Figure 4.3: The calibrated dispersion coefficient of the Rhine Alarm Model increases in magnitude as one goes downstream, i.e. from left to right

Figure 4.4 further shows how the skewness of the pollutant wave increases as one moves downstream. These are based on tracer experiments done in 1989 along the river Rhine. The wave is more skewed early on, e.g. in Maximiliansau, along the river but appears symmetric as passes through Lobith, located further downstream. This confirms the expectation presented in Figure 3.12 in the previous section.

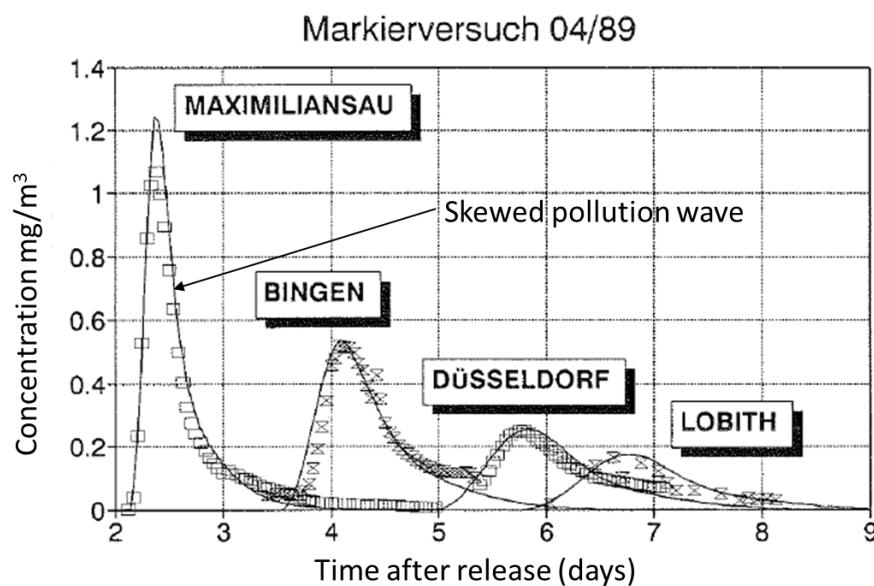


Figure 4.4: The calibrated dispersion coefficient of the Rhine Alarm Model increases in magnitude as one goes downstream, i.e. from left to right

4.3. Adapting the model to different reaches

Note that the Rhine Alarm Model is a modified solution to an Advection Dispersion with decay equation for a reach with a uniform cross-section area. So how can such a model operate in the real world, when the river Rhine changes its cross section area and accumulates more water as the river flows downstream?

In order adapt the simple equation to changing cross sections, we first assume that the river changes its cross-section area in a piece-wise manner. That is, it remains constant for a certain length, then changes and so on. Then the equation for the wave, going from one cross section to another, is changed to a form as if the cross section area was the same as the second reach. Figure 4.5 illustrates the concept.

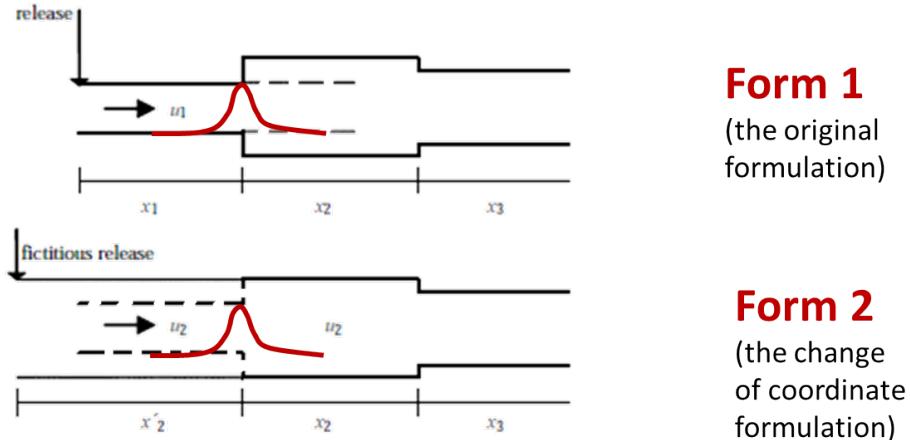


Figure 4.5: Adapting the Rhine Alarm Model equation in form 2, in the second row, at the intersection of the first and the second reach as if the reach never changed

The idea in form 2 is to reshape reach 1 as an extension of reach 2, and shifting the location of the loading, such that peak concentration at the intersection of reach 1 and reach 2 in form 1 remains the same as the peak concentration at the same location in form 2.

This means that instead of loading at distance x_1 from the intersection of the first two cross sections in form 1, the release is extended back by distance x'_2 with the extended reach having the same reach characteristics as reach 2 (i.e. same area of cross section and same velocity u_2). Equating the peak concentrations in form 1 and form 2 at the same location, we obtain:

$$\begin{aligned} C_{\text{form1}}^{\max} &= \frac{m_p}{A_1 2\sqrt{\pi D_1 t_1}} \\ C_{\text{form2}}^{\max} &= \frac{m_p}{A_2 2\sqrt{\pi D_2 t'_2}} \end{aligned} \quad (4.2)$$

where m_p is the load dumped at the point of release. Note that form 2 is fictitious and Equation 4.2 gives equivalence between times and distances in forms 1 and 2. Using Equation 4.2,

$$t'_2 = \left(\frac{A_1}{A_2}\right)^2 \frac{D_1}{D_2} t_1 \quad (4.3)$$

$$\Rightarrow \frac{x'_2}{u_2} = \left(\frac{A_1}{A_2}\right)^2 \frac{D_1}{D_2} \frac{x_1}{u_1} \quad (4.4)$$

In case if there is freshwater flowing in at the point where cross sections change then the pollutant gets diluted. So does its peak, which means that if volumetric flow rate changes from Q_1 in reach 1 to Q_2 in reach 2 then from equation 4.2 we have,

$$C_{\text{form1}}^{\max} Q_1 = C_{\text{form2}}^{\max} Q_2 \quad (4.5)$$

Which would then mean that Equations 4.3 and 4.4 will change to:

$$\begin{aligned} t'_2 &= \left(\frac{Q_2}{Q_1}\right)^2 \left(\frac{A_1}{A_2}\right)^2 \frac{D_1}{D_2} t_1 \\ \Rightarrow \frac{x'_2}{u_2} &= \left(\frac{Q_2}{Q_1}\right)^2 \left(\frac{A_1}{A_2}\right)^2 \frac{D_1}{D_2} \frac{x_1}{u_1} \end{aligned}$$

Let distance and time in form 2 be denoted by \tilde{x} and \tilde{t} respectively. The Rhine Alarm Model equation in form 2 is represented by,

$$c(\tilde{x}, \tilde{t}) = \frac{m_p}{A_2 2 \sqrt{\pi D_1 \tilde{t}}} \exp^{-\frac{(\tilde{x}-u_2 \tilde{t})^2}{4 D_2 \tilde{t}}} \quad (4.6)$$

Further, distance \tilde{x} in form 1 is $x + x'_2 - x_1$ in form 2. Time \tilde{t} in form 1 then is $t + \frac{x'_2}{u_2} - \frac{x_1}{u_1}$ in form 2. In both the cases, x'_2 can be expressed in terms of Equation 4.4. Thus, the Rhine Alarm Model equation in form 2 in Equation 4.6 can be expressed as,

$$c(x, t) = \frac{m_p}{A_2 2 \sqrt{\pi \left[D_2 \left(t - \frac{x_1}{u_1} \right) + D_1 \left(\frac{Q_2}{Q_1} \right)^2 \left(\frac{A_1}{A_2} \right)^2 \frac{x_1}{u_1} \right]}} \exp^{-\frac{(x-x_1)-u_2(t-\frac{x_1}{u_1})^2}{4[D_2(t-\frac{x_1}{u_1})+D_1(\frac{Q_2}{Q_1})^2(\frac{A_1}{A_2})^2\frac{x_1}{u_1}]}} \quad (4.7)$$

Note that this equation is applicable for the rest of reach 2, i.e. for $x'_2 \leq x \leq x_2$. For the third reach, the equation will need to be reformulated again just as it has been done for reach 2.

Repeating the process, the concentration in the j^{th} reach can be given by,

$$c_j(x, t) = \frac{m_p}{A_j \sqrt{4\pi [D_j T_j + P_j]}} \exp^{-\frac{(x_j-u_j T_j)^2}{4(D_j T_j + P_j)}} \quad (4.8)$$

where, $X_j = x - \sum_{n=1}^{j-1} x_n$, $T_j = t - \sum_{n=1}^{j-1} \frac{x_n}{u_n}$ and $P_j = u_j^2 \sum_{n=1}^{j-1} \left(D_n \frac{x_n}{u_n^2} \right)$

Bibliography