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Water quality basics

HYDROEUROPE

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WP4: Accidental Water Pollution

Case Study: Var river (France)

Basic principles and considerations for water quality modelling

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1 Introduction

This teaching material is an integral component of the instructional unit on “Accidental Water Pollution.” This document elucidates the fundamental principles and essential knowledge about water quality, pollution, and modelling. It delineates the primary characteristics of water pollution in aquatic environments and the processes that precipitate this condition. Concurrently, it illustrates water quality modelling and the application of such tools in assessing impacts and formulating strategies for warning systems.

2 Accidental water pollution in the rivers

2.1 About water pollution

The contamination of aquatic ecosystems, such as lakes, rivers, seas, and groundwater, is referred to as water pollution. This happens when contaminants enter water bodies directly or indirectly without being sufficiently treated to eliminate dangerous materials.

Water pollution has a significant effect on aquatic plants and animals. It disturbs large biological communities in addition to affecting specific species and populations. The results are frequently negative, resulting in a reduction in ecosystem health and biodiversity.

Water resource management policies at all levels, from international frameworks to local aquifers and wells, must be continuously assessed and revised due to the serious worldwide problem of water contamination. When anthropogenic pollutants contaminate water to the point where it is unfit for human eating or other uses, the water is considered polluted. Natural occurrences like earthquakes, storms, algae blooms, and volcanic eruptions can also drastically change the ecological state of aquatic ecosystems and the quality of the water.

2.2 The policy setting

By 2015, all water bodies, including marine waters up to one nautical mile off the coast, must have satisfactory qualitative and quantitative status, according to the EU Water Framework Directive (Directive 2000/60/EC). According to the directive, "surface water status" refers to a thorough assessment of a surface water body's condition based on the lesser of its chemical and ecological status.
A surface water body must have at least "good" ecological and chemical state in order to be considered to have "good surface water status." The quality of the composition and operation of aquatic ecosystems in surface waters, including its biological, hydromorphological, and physicochemical components, is referred to as ecological status.

2.3 Types of pollution of water bodies

Despite their interdependence, surface water and groundwater have frequently been examined and treated as distinct resources. Groundwater is created when surface water percolates through the earth. On the other hand, surface water sources can also be nourished by groundwater. Based on where they come from, surface water contamination sources are typically divided into two groups.

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Point Source (PS) - Contaminants that enter a waterway from a single, distinguishable source, like a pipe or ditch, are referred to as point source water pollution. Discharges from factories, sewage treatment plants, and city storm drains are a few examples of sources falling under this category.
Non-point source (NPS) Diffuse contamination that does not come from a single, distinct source is referred to as pollution. NPS contamination is frequently the result of little amounts of pollutants collected over a wide region building up over time. The leaching of nitrogen molecules from fertilized agricultural soils is a typical example. Another example of NPS pollution is the nutrient runoff in storm water from "sheet flow" across a forest or agricultural area.
Sometimes, urban runoff—contaminated storm water that is washed off of roads, highways, and parking lots—is categorized as NPS pollution. This runoff is a point source, though, and is usually directed into storm drain systems before being released into nearby surface waterways via pipes. However, such water is a nonpoint source when it drains straight to the ground without being channeled.

Figure 1: Pollution based on their origin

The specific contaminants contributing to water pollution encompass a broad range of chemicals, pathogens, and physical or sensory alterations such as elevated temperature and discoloration. While many regulated chemicals and substances may occur naturally (e.g., calcium, sodium, iron, manganese), their concentration is crucial in distinguishing between natural components of water and contaminants.

Elevated concentrations of naturally occurring substances can adversely affect aquatic flora and fauna. Oxygen-depleting substances may include natural materials, such as plant matter (e.g., leaves and grass), as well as anthropogenic chemicals. Other natural and human-made substances can cause turbidity, which obstructs light penetration, disrupts plant growth, and clogs the gills of certain fish species.

Many chemical substances are toxic, and pathogens can induce waterborne diseases in human and animal hosts. Alterations in the physical chemistry of water include changes in pH (acidity), electrical conductivity, temperature, and eutrophication.

Eutrophication refers to an increase in the concentration of chemical nutrients in an ecosystem, leading to enhanced primary productivity. Depending on the extent of eutrophication, subsequent negative environmental effects such as anoxia (oxygen depletion) and significant reductions in water quality may occur, impacting fish and other animal populations.

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Figure 2: Muddy River polluted sediment (source: https://ceds.org/muddywatersolutions/)

Figure 3: Polluted River (source: https://www.activesustainability.com/water/causes-consequences-water-pollution/)

2.4 Different groups of pollutants

The two main groups are dominant:

1. Oxygen-**depleting** substances: organic waste, used by aerobic microorganisms in presence of oxygen. Deficit of oxygen in water – if the concentration of oxygen in water is insufficient, oxygen consumed by living creations can go out.

   Very important to know what is the biochemical oxygen demand (BOD). The BOD_5 value is the most expressed in milligrams of oxygen consumed per liter of sample during 5 days of incubation at 20°C and is often used as a robust surrogate of the degree of organic pollution of water.

2. **Water soluble inorganic substances**: salts, acids, compounds of heavy metals. Acidity caused by industrial discharges (especially sulfur dioxide from power plants). Presence in soil (via polluted water) of these substances reduces agricultural harvest, as well as arouses corrosion of the metals.
3. **Inorganic nutrients for plants**: water-soluble nitrates, and phosphates, which are promoters of eutrophication. Ammonia from food processing waste

4. **Organic substances**: oil products, petrol, plastic, pesticides, solvents, detergents, *etc.* In surface and ground waters of developed countries at least **700 synthetic organic substances** – many of them might bring on a kidney illness, hereditary defects, and several cancer varieties.
5. **Suspended substances**: water non-soluble soil or mineral participles, other organic and inorganic substances**.** These substances:
   - cause turbidity,
   - reduce water plant's ability for photosynthesis,
   - affect tropical chains,
   - make difficult for some species to find food,
   - through sediments destroy feeding and spawn territories, as well as, fill the bottom of rivers and lakes, change the flow of rivers,
   - absorb and transport bacteria, pesticides, or other hazardous substances on the surface of solid participles.
6. **Radioactive substances**: Water-soluble radioisotopes can accumulate and move from one to another species in tropical chains. **Ionized radiation of radioactive substances can induce hereditary defects, to bring on cancer illness, and to damage genetic information.**
7. **Heat**: the warm water, as a result of the cooling processes (thermoelectric plants) is flown into a river or lake. Temperature rising lowers the solubility of oxygen in the water and reduces the concentration of oxygen in the water. Wherewith water living species feel a deficit of oxygen and become more sensitive to diseases, parasitic species, and toxic chemicals.
8. **Pathogenic organisms**: microorganisms, parasitic worms. The majority of microorganisms are not dangerous but take part in processes of destruction of the organic substances. Unfortunately, in waters, especially, in wastewater, can be pathogenic microorganisms, which induce infection diseases.

3 Water quality modelling

Water Quality: Refers to the physical, chemical, and biological characteristics of water that determine its suitability for various uses, including drinking, recreation, and habitat.

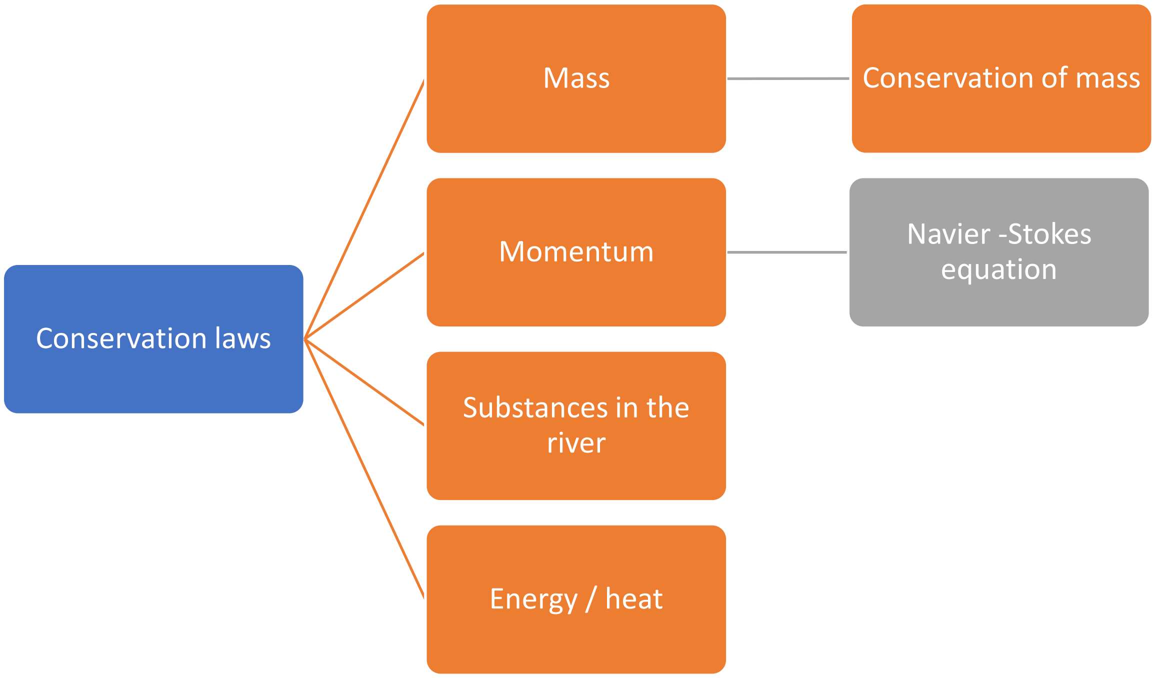
Modeling Purpose: To simulate the behavior of pollutants in rivers, assess environmental impacts, and support regulatory compliance.

The fate of pollutants and the condition of specific water quality variables in bodies of water are simulated using water quality models. includes a range of physical, chemical, and biological processes that regulate the movement and change of these variables, as well as light attenuation coefficients, temperature, wind speed, solar radiation, and pH. Every water quality model, including watershed pollution loading, has unique requirements and characteristics. Some models are applicable to multiple types of water bodies, while others are specific to a single water body.

Water quality is modeled by one or more of the following formulations:

- Advective transport formulations;
- Dispersive transport formulation;
- Heat budget formulation;
- Dissolved oxygen saturation;
- Reaeration
- Carbonaceous deoxygenation, Sediment, BOD, pH, Alkalinity, Nutrients, Algae, Microorganism etc

3.1 Considerations



$\frac{\partial(\rho V_x)}{\partial x}+\frac{\partial(\rho V_y)}{\partial y}+\frac{\partial(\rho V_z)}{\partial z}=-\frac{\partial \rho}{\partial t}$ - Mass balance equation in control volume fixed in space with the density $\rho=\rho(x,y,z)$ and the velocity $V=V(x,y,z)$.

For incompressible fluids (where $\rho = const \ \ => \frac{\partial \rho}{\partial t}=0)\ \frac{\partial V_x}{\partial x}+\frac{\partial V_y}{\partial y}+\frac{\partial V_z}{\partial z}=div\,\vec{V}=0$

3.2 Use of water quality models

The water quality models typically forecast potential outcomes and are often a useful tool for planning, Environmental Impact Assessment (EIA), developing pollutant risk maps for a new plant's intake, master planning, various climate impact scenarios, environmental monitoring and management programs, real-time advisory, oil and chemical spills, beach water quality, aquaculture operations, etc.

Water quality models consist of:

- Transport
- Processes
- Source terms

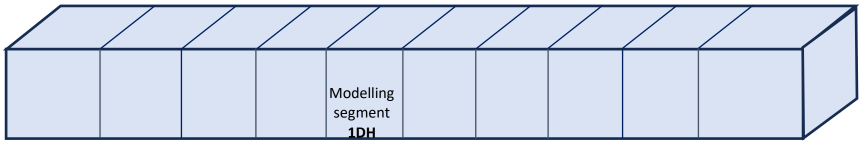
In addition, models have two primary components: beginning conditions and boundary conditions. The choice of model domain is crucial since boundary circumstances have an impact on the model spatially. However, because the beginning conditions affect the model over time, it is best to run the model until a steady state is established before using the data for evaluation.

$M_i^{t+\Delta t}=M_i^t+\Delta t\left(\frac{\Delta M}{\Delta t}\right)_{Tr}+\Delta t\left(\frac{\Delta M}{\Delta t}\right)_P+\Delta t\left(\frac{\Delta M}{\Delta t}\right)_S$ – Mass balance equation

The mass of pollutant in the model segment in the next time step is a function of:

- Current mass (Mi)

- Transport (Tr)
- Processes (P) – the processes can be physical, or chemical. biological for WQ
- Adding/subtraction by sources/sinks (S)



$$M_i^{t+\Delta t} = M_i^t + \Delta t \left(\frac{\Delta M}{\Delta t}\right)_{Tr} + \Delta t \left(\frac{\Delta M}{\Delta t}\right)_P + \Delta t \left(\frac{\Delta M}{\Delta t}\right)_S$$

Sources / discharges
- River discharges
- Incidental spills
- Atmospheric deposition
- Boundary flows

Transport from segment to segment

Processes
- Physical: reaeration, settling, light reflection
- Chemical: mineralisation of organic matter, phosphate adsorption
- Biological: primary production by algae, mortality of bacteria

4 The role of mathematical modeling

the use of mathematical simulation tools to forecast water contamination. A collection of formulas that depict the physical processes that establish the position and momentum of contaminants in a body of water make up a standard water quality model.

Models for certain elements of the hydrological system, like surface runoff models, are available. Models for ocean and estuarine applications, as well as those that deal with hydrologic transport.

In order to create a water quality model, two subsystems must be constructed: one for the water body's hydraulics (volume balance), and another that describes the chemical, physical, and biological processes as well as the transport mechanisms (**advection, diffusion, and dispersion**) that cause variations in the concentration of the water quality variables.

When creating a model, a river channel is separated into control volumes (CV) of length Δx, each of which has two sub-systems: a quality component and a hydrodynamic model. The flow rate out of the CV is equal to the sum of the flow rates into the CV (flow rate from the upstream CV plus flow rate from sources of pollution) less the flow rate of the water sinks (pumping stations) in order to maintain volume balance under steady-state conditions. This formula is:

$$\boldsymbol{Q_i = Q_{i-1} + Q_{f_{p,i}} - Q_{C_{s,i}}}$$

where Q_i is flow rate out of CV *i* and flow rate into downstream CV *i+1* (L^3/T); Q_{i-1} is flow rate into CV *i* and flow rate of upstream CV *i+1* (L^3/T); $Q_{f_{p,i}}$ is flow rate from sources of pollution into CV *i* (L^3/T) and $Q_{C_{s,i}}$ is the flow rate of water pumped out of *i* (L^3/T).

As the river system goes through kinetic processes and mass transfer reactions, the concentration of the contaminants entering it may rise or fall.

The processes of advection and dispersion define the transport of pollutants in the river. Water flow controls effective transfer. Disparities in concentration lead to dispersive transport. The river's physical, chemical, and biological processes and features all have a role.

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The study's goals, the data that is available, the features of the river system, the model's features, and the literature review should all be taken into consideration while choosing a model. It should be chosen in such a way that it covers every significant facet of that specific body of water.

A very simple model could produce ambiguous and erroneous results, whereas a model that is overly complicated could incorporate too many parameters and increase resource costs. Based on its intended usage, the chosen model ought to be approved by the water quality management decision-makers. Each model can simulate specific variables differently. The model's capacity to be updated and incorporate more factors for future requirements should be taken into consideration, and the availability of water quality data for the input variables needed would be crucial for model selection.

Choosing a complete model that can replicate both current and future needs is more economical (Loucks & Van Beek 2017).A very simple model could produce ambiguous and erroneous results, whereas an overly complicated model could incorporate too many parameters and increase resource costs. Based on its intended usage, the chosen model ought to be approved by the water quality management decision-makers. Each model can simulate specific variables differently. The model's capacity to be updated and incorporate more factors for future requirements should be taken into consideration, and the availability of water quality data for the input variables needed would be crucial for model selection. Choosing a complete model that can replicate both current and future needs is more economical (Loucks & Van Beek 2017).

4.1.1 Main processes in water quality modelling

Advection is the process by which the movement of water transports pollutants. Advection is driven by the velocity of the flow in the river. For example, if a river is flowing rapidly, any pollutants or sediments in the water will be carried downstream. The transport is typically in the direction of the flow. If you think of a river carrying leaves downstream, that's advection in action.

Key Concepts:

Flow Velocity (u): The speed at which water flows.

Concentration (C): The amount of pollutant per unit volume of water.

Advection Equation: $\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0$ describes the advection of pollutants.

(C) = Concentration of the pollutant.

(t) = Time.

(x) = Distance along the flow direction.

Diffusion is the process by which particles spread from areas of high concentration to areas of low concentration due to random molecular motion. It occurs naturally and is driven by concentration gradients. Key characteristics are:

- Random Movement: Diffusion occurs due to the random motion of molecules. Even in still water, particles will eventually spread out over time.
- Concentration-Driven: It doesn't require fluid movement; it depends on the concentration difference. For example, if you drop a dye into still water, it will gradually spread out until evenly distributed.

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Diffusion equation $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$ is represented by Fick's second Law. Fick's Law $J = D\frac{\partial C}{\partial x}$ where **(J)** is diffusive flux, **(D)** is diffusive coefficient and $(\frac{\partial C}{\partial x})$ is concentration gradient (second spatial derivative of concentration). Diffusion Coefficient (D): A measure of how quickly a substance spreads through another medium.

Dispersion combines elements of both advection and diffusion. It describes the spreading of particles due to both the bulk motion of the fluid and the random motion of the particles within it. It describes how pollutants spread out in water due to molecular diffusion and turbulent mixing. This process is critical for understanding how pollutants dilute over time and distance. Key Characteristics:

- Combines Effects: Dispersion accounts for how pollutants are transported by flow (like advection) while also considering how they spread out over time (like diffusion).
- Environmental Relevance: Dispersion is particularly important in water quality modeling because it reflects the reality of how contaminants behave in a flowing medium like a river, where both flow and mixing processes occur.

Combined Advection-Diffusion Equation:

When both advection and dispersion are considered, the governing equation becomes:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} - \alpha C$$

Where: α is a decay rate (representing processes such as biodegradation).

5 Modelling software's for water quality

5.1.1 MIKE11

It was first created in 1972 by the Danish Hydraulic Institute in the Netherlands (DHI 1993). The MMIKE-11, MMIKE-21, MMIKE-3, MMIKE SHE, Mouse, and MMIKE Basin models are among the models that have been created (DHI 1996b, 1996a).

Unsteady-state flow in a river system can be simulated using this deterministic model. Both basic and complicated river systems can use it. It can be applied as a WQM to ascertain how discharges affect the quality of river water. It can also be applied to flood studies as a hydraulic model. The model incorporates several modules, such as hydrodynamic, advection-dispersion, and rainfall-runoff.

The concept is frequently used for managing urban pollution in the United Kingdom (UK). The Environment Protection Agency has adopted it to assess the pollutant load of receiving water bodies as a result of wastewater discharge (DHI 2017, 2022).

BOD, DO, nitrate, ammonia, heavy metals, and coliform bacteria are among the water quality metrics that it can mimic.

Water quality, cross-section, hydrodynamic, advection, and dispersion parameters, and boundary conditions defining tributaries, discharges, and abstractions comprise the model's inputs. The information is connected to a flow and water quality time series that is entered into an editor interface (DHI 2017).

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Governing equations

The hydrodynamic model of MIKE-11 uses **Saint-Venant equations** for the simulation of one-dimensional dynamic flows in the rivers as follows.

$$\frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = q$$

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(\alpha \frac{Q^2}{A}\right) + gA\frac{\partial h}{\partial x} + \frac{n^2 gQ|Q|}{AR^{\frac{4}{3}}} = 0$$

where Q is the discharge (m^3/s), A is the cross-section (flow) area (m^2), q is the lateral inflow (m^2/s), h is the water level above a reference datum (m), x is the downstream direction (m), t is the time (s), n is the Manning's resistance coefficient ($s/m^{1/3}$), R is the hydraulic or resistance radius (m), g is the acceleration due to gravity (m^2/s), is the momentum distribution coefficient introduced to account for the nonuniform vertical distribution of velocity in a given section.

For the model to function, a lot of data is needed; otherwise, some constituents may find simulation challenging. For model setup, a skilled individual is needed. The denitrification process is not included in the model, but it can be used for complicated water systems. Because channel cross-sections are necessary to reach boundaries, the simulation takes a long time (Cox 2003; Olowe & Kumarasamy 2018).

Advection/Dispersion Equation $\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} - \alpha C$ where α is the decay rate of the pollutant

Data needed for MIKE 11 water quality model:

- Steady or unsteady flow simulation set up
- Setting up WQ Eco -Lab editor

5.1.2 HEC-RAS

One-dimensional steady flow hydraulics, one- and two-dimensional unsteady flow river hydraulics calculations, quasi-unsteady and full unsteady flow sediment transport-mobile bed modeling, water temperature analysis, and generalized water quality modeling (nutrient fate and transport) can all be done with the U.S. Army Corps of Engineers' River Analysis System (HEC-RAS).

The purpose of the modeling system's water quality analysis component is to enable the user to conduct evaluations of riverine water quality. Algae, dissolved oxygen, carbonaceous biological oxygen demand, dissolved orthophosphate, dissolved organic phosphorus, dissolved ammonium nitrate, dissolved nitrite nitrogen, dissolved nitrate nitrogen, and dissolved organic nitrogen are among the few water-quality constituents that can be transported and subjected to detailed temperature analysis using the current version of HEC-RAS. Upcoming iterations of the program will incorporate the

Governing equations

The mass balance equation, which characterizes a change in mass (or energy) within a control volume as flux into and out of a control volume (mass transport) and external gains or losses (sources and sinks), was employed by the editor for water quality analysis in HEC-RAS.

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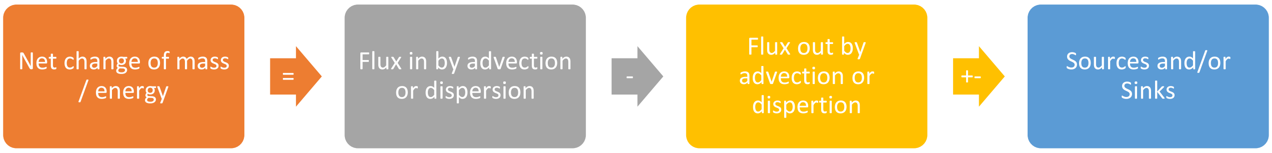

The concentration of mass or heat is the state variable for advection-diffusion. The mass concentration is often the water quality state variable.

Continuity equation $\frac{\partial Q}{\partial t} + \frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x}$=0

Advection/Dispersion equation $\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}$

Data needed for HEC-RAS water quality model:

- Steady or unsteady flow simulation set up
- Parameters for water quality data
- Meteorological data

5.2 Example problem

A pollutant is introduced into a river at a constant rate at position (x = 0). The flow velocity of the river is (u = 1 m/s), and the dispersion coefficient is (D = 0.1 m^2/s). We want to calculate the concentration (C(x,t)) at a position (x = 10 m) downstream after (t = 5 s).

Step-by-Step Solution

Advection-Dispersion Equation: $\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}$

Initial and Boundary Conditions:

Initial condition: (C(x,0) = 0) (no pollutant initially).
Boundary condition: A constant concentration (C_0) is introduced at (x = 0).

Solution Approach:
The solution to the advection-dispersion equation for a continuous point source can be expressed as:

$$C(x,t) = \frac{C_0}{\sqrt{4\pi \cdot D \cdot t}} \exp\left(-\frac{(x-ut)^2}{4Dt}\right)$$

Substitute Given Values:

- (C_0): Assume (C_0 = 1 mg/L (for simplicity).
- (x = 10 m)
- (t = 5 s)
- (u = 1 m/s)
- (D = 0.1 m^2/s)

Then:

$$C(10{,}5) = \frac{1}{\sqrt{4\pi \cdot 0.1 \cdot 5}} \exp\left(-\frac{(10 - 1 \cdot 5)^2}{4 \cdot 0.1 \cdot 5}\right)$$

$$C(10{,}5) = \frac{1}{2.506}\exp(-12.5)$$

$$C(10{,}5) \approx \frac{1}{2.506} \times 3.726 \times 10^{-6} \approx 1.486 \times 10^{-6} \text{ mg/L}$$

After 5 seconds, the concentration of the pollutant at a position 10 meters downstream is approximately (1.486×10^{-6} mg/L). This example illustrates how the advection-dispersion equation can be used to predict pollutant concentration over time and distance in a river system.

Table 1: Calculation table for concentration over time

Time (s)	Concentration (mg/L)	Time (s)	Concentration (mg/L)
0.1	2.9836E-215	5	0.002688734
0.2	7.9039E-107	5.1	0.003238944
0.3	1.00231E-70	5.2	0.003873178
0.4	1.08178E-52	5.3	0.004599619
0.5	6.96698E-42	5.4	0.005426696
0.6	1.10077E-34	5.5	0.006363039
0.7	1.50798E-29	5.6	0.007417444
0.8	1.06421E-25	5.7	0.008598832
0.9	1.04084E-22	5.8	0.009916208
1	2.55419E-20	5.9	0.011378627
1.1	2.29416E-18	6	0.01299515
1.2	9.70026E-17	6.1	0.014774808
1.3	2.29812E-15	6.2	0.01672657
1.4	3.45459E-14	6.3	0.018859306
1.5	3.60952E-13	6.4	0.021181756
1.6	2.80682E-12	6.5	0.023702498
1.7	1.71154E-11	6.6	0.026429924
1.8	8.52326E-11	6.7	0.029372208
1.9	3.5793E-10	6.8	0.032537288
2	1.30047E-09	6.9	0.035932843
2.1	4.17372E-09	7	0.039566272
2.2	1.20348E-08	7.1	0.043444677
2.3	3.16176E-08	7.2	0.047574851
2.4	7.6572E-08	7.3	0.051963264
2.5	1.72631E-07	7.4	0.056616049
2.6	3.6532E-07	7.5	0.061538997
2.7	7.30811E-07	7.6	0.066737549
2.8	1.3904E-06	7.7	0.072216791
2.9	2.52896E-06	7.8	0.077981449
3	4.41749E-06	7.9	0.084035888
3.1	7.43956E-06	8	0.09038411

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3.2	1.21214E-05	8.1	0.097029757
3.3	1.91647E-05	8.2	0.103976113
3.4	2.94818E-05	8.3	0.111226104
3.5	4.4232E-05	8.4	0.118782304
3.6	6.48573E-05	8.5	0.126646941
3.7	9.31177E-05	8.6	0.134821901
3.8	0.000131125	8.7	0.143308736
3.9	0.000181371	8.8	0.15210867
4	0.000246755	8.9	0.16122261
4.1	0.000330607	9	0.170651148
4.2	0.000436697	9.1	0.180394577
4.3	0.000569256	9.2	0.190452895
4.4	0.000732971	9.3	0.200825819
4.5	0.00093299	9.4	0.211512789
4.6	0.001174915	9.5	0.222512983
4.7	0.001464787	9.6	0.233825325
4.8	0.001809073	9.7	0.245448495
4.9	0.00221464	9.8	0.257380938
5	0.002688734	9.9	0.269620878
		10	0.282166324

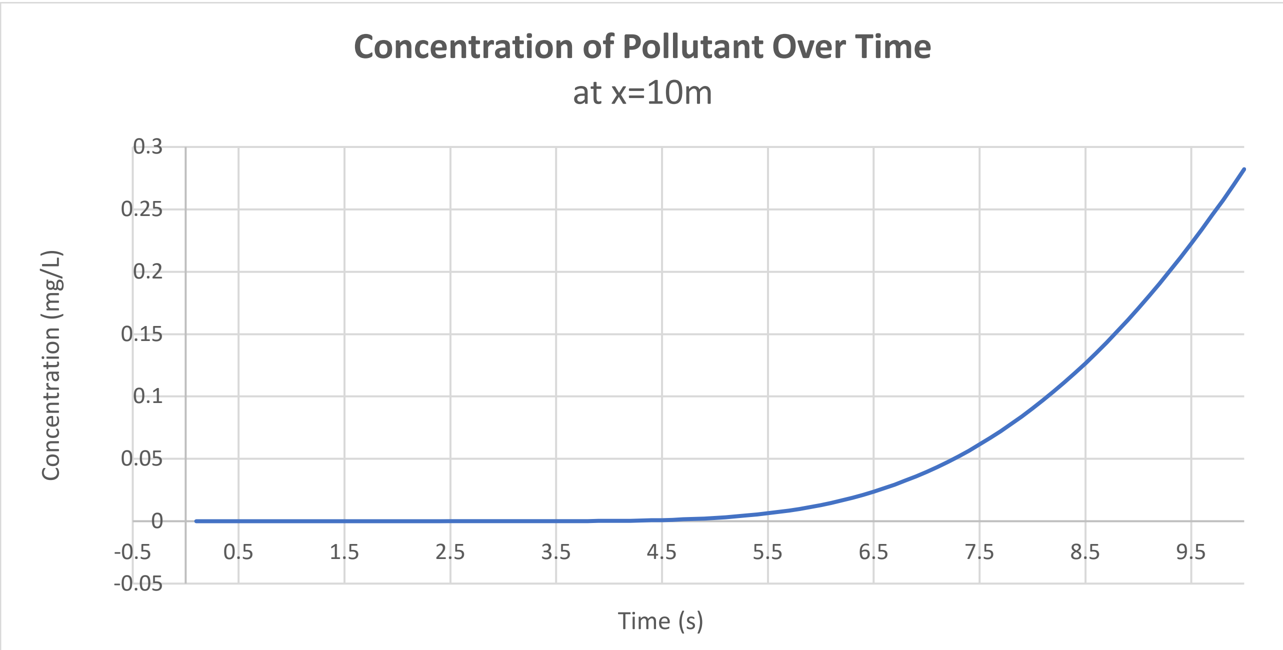

Figure 4: Concentration of pollutant over time at distance of 10m

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