

# **LECTURE 1**

# **MODELLING AND MATHEMATICAL MODELS**

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# **COUSE OUTLINE**

- 1. What is model?
- 2. What is environmental modelling?
- 3. Role of environment modelling
- 4. Types of models
- 5. Mathematical models?





### **1. WHAT IS MODEL?**

A Model is a simplification of reality that is constructed to gain insights into select attributes of a physical, biological, economic, or social system. A formal representation of the behaviors of system processes, often in mathematical or statistical terms. The basis can also be physical or conceptual (Environment Protection Agency, 2009)





Environmental modelling involves the application of multidisciplinary knowledge to explain, explore and predict the Earth's response to environmental change, both natural and human-induced. (DBW,2018)

2. WHAT IS ENVIRONMENTAL MODELLING ?



## **3. ROLE OF ENVIRONMENT MODELLING**

- Improved understanding of environmental systems.
- Developing scientific understanding through quantitative expression of current knowledge of a system (as well as displaying what we know, this may also show up what we do not know);
- Test the effect of changes in a system;
- Aid decision making, including (i) tactical decisions by managers; (ii) strategic decisions by planners.





# 4. TYPE OF MODELS

## Physical modeling

- Physical modeling is a way of modeling and simulating systems that consist of real physical components. A physical model is a smaller or larger physical copy of an object.
- Spatial analysis and similarity theories are used in this process to ensure that the model results can be extrapolated to the real system with high accuracy.
- Physical modeling is the main approach of scientists in developing basic theories of the natural sciences.







# 4. TYPE OF MODELS

### Empirical models

Empirical models describe observed behaviour between variables on the basis of observations alone and say nothing of process. They are usually the simplest mathematical function, which adequately fits the observed relationship between variables. No physical laws or assumptions about the relationships between variables are required. Empirical models have high predictive power but low explanatory depth, they are thus rather specific to the conditions under which data were collected and cannot be generalized easily for application to other conditions



# 4. TYPE OF MODELS

### Mathematical models

- Mathematical model is a representation of real world problem in mathematical form with some simplified assumptions which helps to understand in fundamental and quantitative way
- Mathematical models are much more common and represent states and rates of change according to formally expressed mathematical rules. Mathematical models can range from simple equations to complex software codes applying many equations and rules over time and space discretization. One can further define mathematical models into different types but most models are actually mixtures of many types or are transitional between types.

Dam model is described by a mathematical model









### **Definition & Meaning**



#### System and boundary

 A system is a set of one or more related objects, which can be a physical entity with specific properties or characteristics. The system is isolated from its surroundings by boundaries, which can be physical or virtual

### Open and Closed, flow/non-flow systems

- A closed system is a system that is completely isolated from its environment.
- An open system is a system that has flows of information, energy, and/or matter between the system and its environment, and which adapts to the exchange.
- When the flow of matter does not cross the boundary (but energy can), the system is called a nonflow system. If the material flow can cross the boundary, the system is called a flow system.





#### \* Variable, parameter

- A variable is a value that changes freely in time and space (a compartment or flow) and a state variable is one which represents a state (compartment). A constant is an entity that does not vary with the system under study, for example, acceleration due to gravity is a constant in most Earth-based environmental models (but not in geophysics models looking at gravitational anomalies, for example).
- A parameter is a value which is constant in the case concerned but may vary from case to case where a case can represent a different model run or different grid cells or objects within the same model.







- Calibration is the iterative process of comparing the model with real system, revising the model if necessary, comparing again, until a model is accepted (validated)
- Validation is a process of comparing the model and its behavior to the real system and its behavior
- Sensitivity analysis is the process of defining how changes in model input parameters affect the magnitude of changes in model output..





## **APPROACHES TO MATHEMATICAL MODEL BUILDING**

## Evaluation of simulation results

#### There are two methods to evaluate model performance

- Graphical method (qualitative)
- Statistical methods (quantitative)
- The calibration model does not represent accurately possibly due to the factors multiply as below:
  - The model is used incorrectly or the model setting is incorrect
  - The model is not suitable for this application
  - Lack of data to describe the real world
  - Measurement data is not reliable









### **APPROACHES TO MATHEMATICAL MODEL BUILDING**

### Evaluation of simulation results (cont.)

### Statistical method

Correlation coefficient formulas  $R^2$  are used to find how strong a relationship is between observed and simulate data.

$$R^{2} = \frac{\sum_{i=1}^{n} (Y_{i}^{obs} - \overline{Y}^{obs}) (Y_{i}^{sim} - \overline{Y}^{sim})}{\sqrt{\sum_{i=1}^{n} (Y_{i}^{obs} - \overline{Y}^{obs})^{2}} \times \sqrt{\sum_{i=1}^{n} (Y_{i}^{sim} - \overline{Y}^{sim})^{2}}}$$

 $\overline{Y}^{obs}$ : average value of the series of observed data  $\overline{Y}^{sim}$ : average value of the series of simulated data





### **APPROACHES TO MATHEMATICAL MODEL BUILDING**

### Statistical method

**Nash – Sutcliffe (NSE ):** is a normalized statistic that determines the relative magnitude of the residual variance compared to the measured data variance (Nash and Sutcliffe, 1970). Nash-Sutcliffe efficiency indicates how well the plot of observed versus simulated data fits the 1:1 line. NSE = 1, corresponds to a perfect match of the model to the observed data. NSE = 0, indicates that the model predictions are as accurate as the mean of the observed data, Inf < NSE < 0, indicates that the observed mean is a better predictor than the model.

$$NSE = 1 - \left[ \frac{\sum_{i=1}^{n} (Y_i^{obs} - Y_i^{sim})^2}{\sum_{i=1}^{n} (Y_i^{obs} - \overline{Y}^{obs})^2} \right]$$

Properties	NSE, R <sup>2</sup>	PBIAS	
		Flow	Water - quality
Very Good	0.75 → 1.00	< ± 10 %	<± 25 %
Good	0.65→ 0.75	± 10 % → ± 15 %	± 25 % → ± 40 %
	0.50→0.65	± 15 % → ± 25 %	<mark>± 40 %</mark> → ± 70 %
Unsatisfactory	<0.50	> ± 25 %	> ± 70 %
(Moriasi et al., 2007)			21









# LECTURE 2: INTRODUCTION TO MARINE ENVIRONMENT MODELING

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#### CONTENTS



## Purpose of modelling the marine environmental

# Fundamental quantities

- Mass and Concentration
- Rates

# Mathematical models

- Model Implementations
- Conservations of Mass and the Mass Balance





#### PURPOSES OF MODELLING THE MARINE ENVIRONMENTAL

#### Distribution Load Discharge

- Control the marine environment to achieve a specified environmental quality
- Fishery management and offshores works
- Determining Total Maximum Daily Load (TMDL)
- TMDL Total Maximum Daily Load: the calculation of the maximum amount of a pollutant allowed to enter a waterbody so that the waterbody will meet and continue to meet water quality standards for that particular pollutant. A TMDL determines a pollutant reduction target and allocates load reductions necessary to the source(s) of the pollutant.





#### PURPOSES OF MODELLING THE MARINE ENVIRONMENTAL

### \* Modelling

- Understanding the processes of the transmission of substances to the marine and ocean environment
- Understanding of ecosystem

Understanding of natural system and their reactions to changing conditions.





## FUNDAMENTAL QUANTITIES

## Mass and concentration

- Mass(m): The amount of pollutant in a system
- Concentration(C): conventinally express in metric units.

$$C = \frac{m}{V}$$

C: Concentration [ML-3] m: mass [M]

V: Volume [L<sup>3</sup>]

Some water – quality variables along with typical units

Varibales	Units
Total Disolved solids, salinity	$gL^{-1} \Leftrightarrow kg m^{-3} \Leftrightarrow ppt$
DO, BOD, NO <sub>2</sub>	mgL⁻¹ ⇔ g m⁻³ ⇔ ppm
PO <sup>4</sup> , Chlorophyll a, Toxics	$\mu$ gL <sup>-1</sup> $\Leftrightarrow$ mg m <sup>-3</sup> $\Leftrightarrow$ ppb
Toxics	ngL⁻¹ ⇔ µg m⁻³ ⇔ pptr







### **FUNDAMENTAL QUANTITIES (cont.)**

#### Example 1:

A pond having constant volume and no outlet has a surface area A , of 104  $m^2$  and a mean depth H of 2 m . It initially has a concentration of 0.8 ppm . Two days later a measurement indicates that the concentration has risen to 1.5 ppm

(a) What was the mass loading rate during this time?

(b) If you hypothesize that the only possible source of this pollutant was from the atmosphere, estimate the flux that occurred.







### **MATHEMATICAL MODELS**

Mathematical modes can be represented generally:

C = f (W, physics, chemistry, biology)

→ The cause – effect relationship between loading and concentration depends on the physicals, chemical and biological characteristics of the receiving water.

$$C = \frac{1}{a}W$$

where a = an assimilation factor ( $L^{3}T - 1$ ) that represents the physics , chemistry , and biology of the receiving water . This Equation is called "linear "because c and W are directly proportional to each other . Consequently if W is doubled , c is doubled . Similarly if W is halved , c is halve



#### \* Model Implementation

(a) Simulation mode: the model is used to simulate system response (concentration ) as a function of a stimulus (loading) and system characteristics (the assimilation factor)

$$C = \frac{1}{a}W$$

(b) **Design mode I** (Assimilative capacity)

The model can be rearranged to yield : **W = ac** 

**MATHEMATICAL MODELS** 

This implementation is referred to as a "design "mode because it provides information that can be directly used for engineering design of the system. It is formally referred to as an " assimilative capacity " computation because it provides an estimate of the loading required to meet a desirable concentration level or standard . Thus it forms the basis for wastewater treatment plant design . It should also clarify why a is called an " assimilation factor

(c) Design Mode II (environmental modification)

A second design implementation is  $\mathbf{a} = \mathbf{W}/\mathbf{C}$ . In this case the environment itself becomes the focus of the remedial effort. This equation is formulated to determine how, for a given loading rate, the environment might be modified to achieve the prescribed standard. This type of application is needed when affordable treatment (that is, reduction in W) is not adequate to meet water - quality standards.



### MATHEMATICAL MODELS

#### **Example 2: (ASSIMILATION FACTOR)**

Lake Ontario in the early 1970s had a total phosphorus loading of approximately 10,500 mta (metric tonnes per annum, where a metric tonne equals 1000 kg) and an in - lake concentration of 21  $\mu$ g/L. In 1973 the state of New York and the province of Ontario ordered a reduction of detergent phosphate content. This action reduced loadings to 8000 mta.

(a) Compute the assimilation factor for Lake Ontario?

(b) What in - lake concentration would result from the detergent phosphate reduction action ?

( c ) If the water - quality objective is to bring in - lake levels down to 10 μg L<sup>-1</sup>, how much additional load reduction is needed ?



## MATHEMATICAL MODELS

#### **Example 2: (ASSIMILATION FACTOR)**

#### Solution:

MARE

(a) The assimilation factor can be calculated as

$$a = \frac{W}{c} = \frac{10,500 \text{ mta}}{21 \mu \text{g/L}} = 500 \frac{\text{mta}}{\mu \text{g L}^{-1}}$$

(b) In - lake levels from the phosphorus reduction can be calculated as:

$$c = \frac{W}{a} = \frac{8000 \text{ mta}}{\frac{1000 \text{ mta}}{1000 \text{ mta}}} = 16 \text{ }\mu\text{g }\text{L}^{-1}$$
(c) W = ac = 500  $\frac{\text{mta}}{1000 \text{ L}^{-1}} \times 10 \text{ }\mu\text{g }\text{L}^{-1} = 5000 \text{ mta}$ 





### **CONSERVATIONS OF MASS AND THE MASS BALANCE**

MOMENTUM



Momentum = Mass \* Velocity

MASS



Water Mass = PV Constituent Mass = VC e = Density, V = Volume, C = Concentration



#### Law of Conservation of Mass

The mass in an isolated system can neither be created nor be destroyed but can be transformed from one form to another (Antoine Lavoisier's 1789)

- Some of Law of Conservation:
  - Mass
  - Momentum

#### - Heat

In quantitative terms the principle is expressed as a mass - balance equation that accounts for all transfers of matter across the system's boundaries and all transformations occurring within the system





### **CONSERVATIONS OF MASS AND THE MASS BALANCE**






#### **CONSERVATIONS OF MASS AND THE MASS BALANCE**

	SYNTHESIS	DECOMPOSITION	NON - REACTIVE
	REACTIONS	REACTIONS	SUBSTANCES
•	Product of chemical	Reactants	• Chloride Cl <sup>-</sup> ,
	reaction	• BOD	Bromide Br
•	The growth of	Radioactive decay	Non-biodegradable
	algae in the water	Sedimentation	organic matter
•	Gas <mark>abso</mark> rption	Decomposition of organic	Metals
•	Chemical	matter	Stable isotopes
	desorption	Chemical adsorption	
		Degasification	
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#### HISTORICAL DEVELOPMENT OF WATER – QUANLITY MODELS

- ✤ 1925-1960: Streeter-Phelps
- 1960-1970: Computerization
- ✤ 1970-1977: Biology
- ✤ 1977 present: Toxics

1925-1960 (streeter-Phelps)
 Problems: untreated and primary effluent
 Pollutants: BOD/DO
 Systems: streams/estuaries (1D)
 Kinetics: linear, feed-forward
 Solutions: analytical

MARE

1960-1970 (computerization)
 Problems: primary and secondary effluent
 Pollutants: BOD/DO
 Systems: estuaries/streams(1D/2D)
 Kinetics: linear, feed-forward
 Solutions: analytical and numerical

1970-1977 (biology)
 Problems: eutrophication
 Pollutants: nutrients
 Systems: lakes/estuaries/streams (1D/2D/3D)
 Kinetics: nonlinear, feedback
 Solutions: numerical

1977 - nay (toxics)
 Problems: Toxics
 Pollutants: organic,m metals
 Systems: Sediment-water interactions/food chain ineteraction (lakes/estuaries/stream)
 Kinetics: linear, equilibrum
 Solutions: numerical and analytical







#### **EXERCISES**

Ex.2.1: A waste source enters a river as depicted in figure below.

- What is the resulting flow rate in m<sup>3</sup>s<sup>-1</sup> (cms)? (a)
- If instantaneous mixing occurs, what is the resulting concentration in ppm? (b)
- where: 1 gallon=3.785 l, 1ft=0.3048 m, 1ft/s=0.3048 m/s.







- Ex. 2.2: I the early 1970s Lake Michigan had a total phosphourus loading 6950 mta (mta: metric tones per annum. Metric tone=1000kg;T.e mta=10<sup>3</sup> kg/year) and an in-lake concentration of 8  $\mu$ g/L
- a) Determine the lake's assimilation factor (km<sup>3</sup>/year)
- b) What loading rate would be required to bring in-lake levels down to approximately 5 µg/L



# --- THE END ----





## LECTURE 3: DYNAMICS CURRENTS AND TIDES

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## CONTENTS



- **\* REACTION FUNDAMENTALS**
- Reaction Types
- Reaction Kinetics
- \* ANALYSIS OF RATE DATA
- The integral Method
- The differential method
- ✤ TEMPERATURE EFFECTS





## **REACTION TYPES**

- Homogeneous reaction: involve a single phase, (that is, liquid, gas, or solid)
- Heterogeneous reaction: involve more than one phase, with reaction usually occurring at the surface between phase
- Irreversible reaction: These proceed in a single direction and continue until the reactants are exhausted.
- Reversible reaction: can proceed in either direction, depending on the relative concentration of the reactants and the products.







## **ZERO-, FIRST AND SECOND – ORDER REACTIONS**

**\* Zero - order**(n = 0)

Equation (\*):  $\frac{dC}{dt} = -k$ 

Where: k has units of ML<sup>-3</sup>T<sup>-1</sup>

If  $C = C_0$  at t =0, then this equation can be integrated by separation of varibales to yield:

$$C = C_0 - kt$$

- A constant rate of depletion per unit time
- Plot of concentration versus time yields a straight line







 $\ln C_0$ 

C **4** 

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### **ZERO-, FIRST AND SECOND – ORDER REACTIONS**

- First order(n = 1)
- Equation(\*):  $\frac{dC}{dt} = -kC$  where k has units of T<sup>-1</sup>

If C = C<sub>0</sub> at t =0, then this equation can be integrated by separation of variables to yield: In c – In  $c_0 = -kt$ 

where  $k' = \frac{k}{2.3025}$ 

Taking the exponential of both sides gives:  $C = C_0 e^{-kt}$ 

- The concentrations decrease following exponential function
- The concentration curve asymptotically approaches zero with time
- Taking te inverse logarithm base e to base -10

$$C = C_0 10^{-k't}$$





## **ZERO-, FIRST AND SECOND – ORDER REACTIONS**

#### Second - order(n = 2)

Equation(\*):

where k has units of L<sup>3</sup>M<sup>-1</sup>T<sup>-1</sup>

 $1/C_0$ 

If  $C = C_0$  at t =0, then this equation can be integrated by separation of variables to yield 1/C

• Plot of 1/c versus t should yield a straight line

 $\frac{1}{C} = \frac{1}{C_{c}} + kt$ 

 $\frac{dC}{dt} = -kC^2$ 

The above equation can also expressed in term of concentration as a function of time by inverting to gives:

$$C = C_0 \frac{1}{1 + kC_0 t}$$





## **ZERO-, FIRST AND SECOND – ORDER REACTIONS**

- ✤ n order (n≠1)
- Equation(\*):  $\frac{dC}{dt} = -kC^n$

If  $C = C_0$  at t =0, then this equation can be integrated by separation of variables to yield

$$\frac{1}{C^{n-1}} = \frac{1}{C_0^{n-1}} + (n-1)kt$$

Plot of 1/C<sup>n-1</sup> versus t should yield a straight line

Solution for c: 
$$C = C_0 \frac{1}{\left[1 + (n-1)kC_0^{n-1}t\right]^{1/(n-1)}}$$

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#### **ANALYSIS OF RATE DATA**

A simple approach is to measuring concentrations in each bottle over time to develop a relationship between concentrations and time.







## **ANALYSIS OF RATE DATA**

#### The integral method:

- Step 1: guessing n
- Step 2: Integrating equation (\*) to obtain a function, C(t)
- Step 3: Graphical methods are then employes to determine whether the model fits the data adequately

Order	Rate units	Dependent y	Independent x	Int <mark>ercep</mark> t	Slope
n=0	M(L <sup>3</sup> T) <sup>-1</sup>	С	t	C <sub>0</sub>	-K
n=1	T-1 '	InC	t	InC	-K
n=2	L <sup>3</sup> (MT) <sup>-1</sup>	1/C	t	1/C <sub>0</sub>	κ
n #1	(L <sup>3</sup> M <sup>-1</sup> ) <sup>n-1</sup> T <sup>-1</sup>	C <sup>1-n</sup>	t	C <sub>0</sub> <sup>1-n</sup>	(n-1)K





## **ANALYSIS OF RATE DATA**

Example 1: Employ the integral method to determine whether the following data is zero-, first, second – order

t (day)	0	1	3	5	10	15	20
C (mg/l)	12	10.7	9	7.1	4.6	2.5	1.8

If any of these models seem to hold, evaluate k and c<sub>o</sub>





#### Solution:

To determine whether the following data is zero-, first, second – order, we will evaluate for each order.







The best-fit line for this case as below: lnC = 2.47 - 0.0972t which  $R^2 = 0.995$ Therefore the estimates of two model parameter are:  $k = 0.0972 \text{ day}^{-1}$   $C_0 = e^{2.47} = 11.8 \text{ mg/l}$ Thus the resulting model is  $C = 11.8e^{-0.0972t}$ 





log

dC<sub>A</sub> dt Co-funded by the Erasmus+ Programme of the European Union

slope = n

CA

00

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## **ANALYSIS OF RATE DATA (cont.)**

### The differential Method

Taking the logarithmic of both sides of Equation(\*), to give:

$$\log\left(-\frac{dC}{dt}\right) = \log k + n\log C$$

Plot of log (-dC/dt) versus log C should yield a straight line with a slope of n and an intercept of log k

**Numerical differentiation:** Finite -Difference approximations to estimate dC/dt.

Centered Differentiation

$$\frac{\mathrm{dC}_{\mathrm{i}}}{\mathrm{dt}} \cong \frac{\Delta \mathrm{C}}{\Delta \mathrm{t}} = \frac{\mathrm{C}_{\mathrm{i+1}} - \mathrm{C}_{\mathrm{i-1}}}{\mathrm{t}_{\mathrm{i+1}} - \mathrm{t}_{\mathrm{i-1}}}$$





## **ANALYSIS OF RATE DATA (cont.)**

#### The differential Method (cont.)

<u>t</u>			t <sub>o</sub>	t <sub>1</sub>	t <sub>2</sub>	$t_3$ $t_4$ $t_5$
С			C <sub>0</sub>	C <sub>1</sub>	C <sub>2</sub>	$C_3$ $C_4$ $C_5$
l ▲ F	ادىتە	aroa	difforor	tistion		Drawing sm <mark>ooth cu</mark> rve that best
V L	quar		unerer	itiation		approximates the area under the
t	С	∆t	ΔC	∆C/∆t	dC/dt	histogram, t <mark>ry to ba</mark> lance out the histogram
t <sub>1</sub>	C <sub>1</sub>				(dC/dt) <sub>1</sub>	areas above and below the drawn curve.
	•	$t_2 - t_1$	$C_2 - C_1$	$(\Delta C/\Delta t)_2$		Then the de <mark>rivative</mark> estimates at the data
t <sub>2</sub>	C <sub>2</sub>	t <sub>3</sub> – t <sub>2</sub>	$C_{3} - C_{2}$	(∆C/∆t) <sub>3</sub>	$(dC/dt)_2$	points can be read directly from the curve. $(\Delta C / \Delta t)_2$
t <sub>3</sub>	C <sub>3</sub>				$(dC/dt)_3$	
4	0	$t_4 - t_3$	$C_4 - C_3$	$(\Delta C/\Delta t)_4$	(-10(-14)	(dC/dt) <sub>2</sub>
t <sub>4</sub>	$C_4$	+ +		(AC/At)	(dC/dt) <sub>4</sub>	$-\Delta C$
<u>t<sub>5</sub></u>	C <sub>5</sub>	ι <sub>5</sub> — ι <sub>4</sub>	<b>U</b> <sub>5</sub> – <b>U</b> <sub>4</sub>		(dC/dt) <sub>5</sub>	∆t
						1 2 3 <b>t</b> 4 5





## **ANALYSIS OF RATE DATA (cont.)**

#### The differential Method (cont.)







## **ANALYSIS OF RATE DATA (cont.)**

Example 2: Use the differential method to evaluate the order and the constant for the data from Example 1. Use equal-area differentiation to smooth the derivative estimates

t (d)	0	1	3	5	10	15	20
C (mg/l)	12	10.7	9	7.1	4.6	2.5	1.8





#### Solution:

#### Determine derivative estimate from time series of concentration

	t	С	-∆C/∆t	-dC/dt	logC	log(-dC/dt)	
	(day)	(mg/l)	mg/	/l/d			
	0	12.0		1.25	1.08	0.1	
			1.3				1.5 $_{ op}$
	1	10.7		1.1	1.03	0.04	
			0.85				
	3	9.0		0.9	0.95	-0.05	
			0.95				
	5	7.1		0.72	0.85	-0.14	
			0.50				
	10	4.6		0.45	0.66	-0.35	
			0.42				
	15	2.5		0.27	0.40	-0.57	0 5 10 15 20
			0.14				t
_	20	1.8		0.15	0.26	-0.82	Equal-area differentiation







### ANALYSIS OF RATE DATA (cont.)

#### ✤ The method of Initial Rates

- There are cases where reactions occur in which complications arise over time. For example a significant reverse reaction might occur. Further some reactions are very slow and the time required for the complete experiment might be prohibitive.
- Using data from the beginning stages of the experiment to determine the rate constant and order
- The differential method

Taking the logarithm of the negative of Eq. (\*):

 $\log\left(-\frac{dC_{0}}{dt}\right) = \log k + n\log C_{0}$ 

Plot log(-dC0/dt) versus  $log(C_o)$  should yield a straight line can be used to estimate k and n, the slope provides an estimate of the order, whereas the intercept provides an estimate logarithm





#### **ANALYSIS OF RATE DATA (cont.)**

#### The method of Half -lives

The half-lives of a reaction is the time it takes for the concentration to drop to one-half of its initial value. In other words.

 $C(t_{50}) = 0.5C_0$ 

If  $C = C_0$  at t =0, then this equation (\*) can be integrated by separation of variables to yield

Combining two equations above to give:

$$E_{50} = \frac{2^{n-1} - 1}{k(n-1)} \frac{1}{C_0^{n-1}}$$

 $t = \frac{1}{kC_0^{n-1}(n-1)} \left| \left( \frac{C_0}{C} \right)^{n-1} - 1 \right|$ 

Taking the logarithm of this equation provides a linear relationship  $\log t_{50}$ 

$$\log_{50} = \log \frac{2^{n-1} - 1}{k(n-1)} + (1 - n)\log C_0$$







## **ANALYSIS OF RATE DATA (cont.))**

#### The method of Half -lives (cont.)

For general case with response time  $t_{\phi}$ , where  $\phi$  is percent reduction:

$$=\frac{\left[\frac{100}{(100-\phi)}\right]^{n-1}-1}{k(n-1)}\frac{1}{C_0^{n-1}}$$





(\*\*\*\*\* \*\*\*\*\*

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The rates of most reaction in natural waters increase with temperature. A more rigorous quantification of the temperature dependence is provided by the Arhenius equation.

 $k(T_a) = Ae^{\frac{-E}{RT_a}} E$  R

a preexponential or frequency factor Activation energy (J.mole<sup>-1</sup>) the gas constant(8.314 J.mole<sup>-1</sup>.K<sup>-1</sup>) absolute temperature (K).

 $\mathbf{k}(\mathbf{T}) = \mathbf{k}(20)\theta^{\mathrm{T}-20}$ 

Compare the reaction rate constant at two different temperatures

$$\frac{k(T_{a2})}{k(T_{a1})} = e^{\frac{E(T_{a2}-T_{a1})}{RT_{a2}T_{a1}}} \qquad T_{a1}.T_{a2} = const$$

$$\theta = e^{\frac{E}{RT_{a2}T_{a1}}}$$

$$\theta = e^{\frac{E}{RT_{a2}T_{a1}}}$$

Compare the reaction rate constant at 20°C:

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## **TEMPERATURE EFFECTS**



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**Example 3:** Evaluation of temperature dependency of reaction. A laboratory provides you with the flowing results for a reaction

 $T_1 = 4^{\circ}C$   $k_1 = 0.12 \text{ ng}ay^{-1}$ 

 $T_2 = 16^{\circ}C$   $k_2 = 0.20 \text{ ngày}^{-1}$ 

(a) Evaluate  $\theta$  for this reaction

(b) Determine the rate at 20°C





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#### **Solution**:

#### (a) Taking the logarithm and raise the results to power of 10 to give

 $logk(T_2) - logk(T_1)$  $T_2 - T_1$  $\theta = 10$ 

Substituting the data gives:

$$\theta = 10^{\frac{\log 0.12 - \log 0.20}{4 - 16}} = 1.0435$$

(b) The rate at 20°C

$$k(20) = 0.20 \times 1.0435^{20-16} = 0.237 \text{ (ngày)}$$



**BÀI TẬP** 



 We design an experiment and determine the oxygen concentration as follows:

t(d)	0	2	5	10	20	30	40	50	60	70
C(mg/l)	10	8.4	6.5	4.4	2.3	1.6	1.3	1.2	1.1	1.1

Determine the order and the rate of the reaction?



# --- THE END ----





#### LECTURE 4: CURRENTS DYNAMICS

Lecturer: Prof. Nguyen Ky Phung MSc. DangThi Thanh Le MSc. Tran Thi Kim








# **Currents classification**



Currents can be classified according to the following basic characteristics:

- According to the factors or forces that driven the currents
- According to stability.
- According to the distribution depth.
- According to the nature of movement.
- According to the physiological nature of the water mass.
- In currents theories, classifying currents by factors or forces that cause currents is considered the main classification.











# **HYDRODYNAMICS**

- Study the movement of the fluid and the forces acting on it.
- Flow modeling relies on three basic factors:
- Partial differential equations representing the laws of physics
- Finite difference diagram for generating systems of algebraic equations
- Algorithms to solve these equations





## **HYDRODYNAMICS (Cont)**



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#### Geometric features of the channel cross section













# **HYDRODYNAMICS (Cont)**



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#### **Saint-Venant equation**

#### Approach

Simplifying actual flow processes in a 1-dimensional problem

- Assumption
- Flow is one-dimensional
- Hydrostatic pressure prevails and vertical accelerations are negligible
- Streamline curvature is small.
- Bottom slope of the channel is small.
- Manning's equation is used to describe resistance effects
- The fluid is incompressible







## --- THE END ----



# **LECTURE**

# **MODELLING THE MARINE ENVIRONMENT**

## Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le







### Lecture 5

## FUNDAMENTAL EQUATIONS DESCRIBING CURRENTS AND BOUNDARY CONDITIONS

Lecturer: Professor. Nguyen Ky Phung Ms. Dang Thi Thanh Le



### **CONTENTS**



#### I. FUNDAMENTAL EQUATIONS DESCRIBING CURRENTS AND BOUNDARY CONDITIONS

- 1.1. Equations of Motion for Perfect and Viscous Fluids
- 1.2. Continuity Equation
- 1.3. Salt Conservation Equation
- 1.4. Seawater State Equation
- 1.5. Turbulent motion, Reynolds stress

**II. CLASSIFICATION OF NON-STOP PROCESSES IN THE OCEAN AND SOME** 

**APPROXIMATIONS APPLIED TO CURRENTS RESEARCH** 



MARE Erasmus+ Programm FUNDAMENTAL EQUATIONS DESCRIBING CURRENTS AND BOUNDARY The state of the liquid is completely determined, if at each point of the liquid at any time completely identified: Pressure P(x,y,z,t);

Density  $\rho(x,y,z,t)$ ,

Velocity with components u(x,y,z,t), v(x, y, z,t), w(x,y,z,t).











Equations of Motion for Perfect and Viscous Fluids

According to the Dalambe principle of the equilibrium of the dx dy dz water particle under the effect of those three forces, we have: dV = D = dV = D = dV

$$\rho dx \cdot dy \cdot dz \cdot \frac{dv}{dt} = \rho \cdot F \cdot dx dy dz + R$$
 (5.1)

Projecting the equation (1.25) onto the coordinate axes and dividing by  $\rho$  (for non-compressible liquids), we have:

$\frac{du}{dt} = X - \frac{1}{\rho} \frac{\partial P}{\partial x} + \upsilon \nabla u$ $\frac{dv}{dt} = Y - \frac{1}{\rho} \frac{\partial P}{\partial y} + \upsilon \nabla v  (5.2)$ $\frac{dw}{dt} = Z - \frac{1}{\rho} \frac{\partial P}{\partial z} + \upsilon \nabla w$	where $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ ; $\upsilon = \text{const}$ is a kinetic coefficient, for perfect liquid: $v = 0$ ; $\frac{du}{dt} = X - \frac{1}{\rho} \frac{\partial P}{\partial x}$
	$\frac{\mathrm{d}\nu}{\mathrm{d}t} = Y - \frac{1}{\rho} \frac{\partial P}{\partial y}$ $\frac{\mathrm{d}w}{\mathrm{d}t} = Z - \frac{1}{\rho} \frac{\partial P}{\partial z}$ (5.3)

Where:  $\frac{a}{dt}$  is the time differential of a definite liquid particle, and the liquid particle's velovcity is a function of both time and space, so we have:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z}$$



the





#### Equations of Motion for Perfect and Viscous Fluids

Therefore the motion equation has form:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = X - \frac{1}{\rho} \frac{\partial P}{\partial x} + \upsilon \nabla u$$
$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = Y - \frac{1}{\rho} \frac{\partial P}{\partial y} + \upsilon \nabla v \qquad (5.4)$$
$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = Z - \frac{1}{\rho} \frac{\partial P}{\partial z} + \upsilon \nabla w$$

Equation (5.4) is the Navie-St. equation for the viscous fluids. For the ideal liquid we have:  $v\nabla u = v\nabla v = v\nabla w = 0$ 

The above equations are nonlinear. We're going to linearize them if we ignore space acceleration. Movement is considered stable (or stop) if the velocity at any given time does not depend on the time or local acceleration:

$$\frac{\partial u}{\partial t} = \frac{\partial v}{\partial t} = \frac{\partial w}{\partial t} = 0$$







Considering the continuity equation of the fluid, i.e. we consider the continuous properties of that fluid. Assuming there is a fluid volume factor  $\delta x \, \delta y \, \delta z$ , consider the volume of liquid entering and exiting this volume during the period  $\delta t$ .

In the direction of the Ox axis, the mass of fluid entering that volume:  $(\rho u)_x \delta t \delta y \delta z$ 

and the mass of fluid that comes out of volume is:  $(\rho u)_{x+\delta x} \delta t \delta y \delta z$ 

So, after the period  $\delta t \, \delta x \, \delta y \, \delta z$  là: Ox axis movement will increase the amount of fluid in the volume factor  $\partial(\rho \cdot u)$ 

$$(\rho \mathbf{u})_{\mathbf{x}} \delta \mathbf{z} \delta \mathbf{y} \delta \mathbf{t} - (\rho \mathbf{u})_{\mathbf{x} + \delta \mathbf{x}} \cdot \delta \mathbf{z} \delta \mathbf{y} \delta \mathbf{t} = -\frac{\partial (\rho \cdot \mathbf{u})}{\partial \mathbf{x}} \delta \mathbf{x} \delta \mathbf{y} \delta \mathbf{z} \delta \mathbf{t}$$

Similarly, in the direction of the Oy axis and the Oz axis we also have:

$$-\frac{\partial(\rho,\mathbf{v})}{\partial \mathbf{y}}\delta\mathbf{x}\delta\mathbf{y}\delta\mathbf{z}\delta\mathbf{t}; -\frac{\partial(\rho\cdot\mathbf{w})}{\partial \mathbf{z}}\delta\mathbf{x}\delta\mathbf{y}\delta\mathbf{z}\delta\mathbf{t}$$



Or



According to the law of mass conservation, the total volume of liquids entering and exiting volume δx δy δz must be by changing the volume of fluid during that time.:

$$\begin{pmatrix} \rho + \frac{\partial \rho}{\partial t} \partial t \end{pmatrix} \delta x \delta y \delta z - \rho \delta x \delta y \delta z = \frac{\partial \rho}{\partial t} \delta t \delta x \delta y \delta z \\ = -\frac{\partial (\rho u)}{\partial x} \delta x \delta y \delta z t - \frac{\partial (\rho v)}{\partial y} \delta x \delta y \delta z \delta t - \frac{\partial (\rho w)}{\partial z} \delta x \delta y \delta z \delta t \\ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0 \\ \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho, V) = 0 \tag{5.5}$$

The equation (5.5) is the continuity equation of compressed liquid. In practical calculations it is common to view liquids as uncompressed  $\rho = \text{const}$ :  $\frac{\partial \rho}{\partial t} = 0$ 

**Continuity equation is constantly in form:** div $V = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$ 





Consider the amount of salt that goes beyond the limits of a volume factor  $\delta x \ \delta y \ \delta z$  follow the Ox axis at a time of ration x during the period  $\delta t$  là  $(S.p.u)_x \ \delta y \delta z \delta t$ . The amount of salt passing through the opposite side is  $(S.p.u)_{x+\delta x} \delta y \delta z \delta t$ .

Therefore, the movement in the direction of the Ox axis has the excess salt.:  $-\frac{\partial(\rho \cdot u.S)}{\partial x}\delta x \delta y z \delta t$ 

In the direction of the axes Oy and Oz also:

$$\frac{\partial(\rho \cdot u.S)}{\partial y} \delta x \delta y \delta z \delta t \quad ; \quad -\frac{\partial(\rho \cdot w \cdot S)}{\partial z} \delta x \delta y \delta z \delta t$$

Order the initial amount of salt in volume  $\delta x \, \delta y \, \delta z \, la \, \rho S. \delta x \, \delta y \, \delta z$ , after  $\delta t$  the amount of salt in the volume factor is:  $\left(\rho \cdot S + \frac{\partial(\rho \cdot S)}{\partial t} \delta t\right) \delta x \delta y \delta z$ According to the law of conservation:  $+ \frac{\partial}{\partial t} (\rho \cdot u \cdot S) + \frac{\partial}{\partial y} (\rho \cdot v \cdot S) + \frac{\partial}{\partial z} (\rho \cdot w \cdot S) = 0$  (5.7) When using continuity equations (1.29) we have:  $\frac{\partial S}{\partial t} + u \frac{\partial S}{\partial x} + v \frac{\partial S}{\partial y} + w \frac{\partial S}{\partial t} = 0$  (5.8) When S(x,y,z) = const, so  $\frac{\partial S}{\partial t} = 0$ , therefore:  $u \frac{\partial S}{\partial x} + v \frac{\partial S}{\partial y} + w \frac{\partial S}{\partial z} = 0$  (5.9) The heat conservation equation is received in the same way.:  $\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = 0$  (5.10)



Seawater is a compressed liquid, i.e. its density changes. The dependence of the specific volume  $\alpha$  and the density of the water on the state parameters: T temperature, S salinity and P pressure are indicated by the state equation. The general form of the state equation is as follows:  $\rho = \rho(T, S, P)$  (5.11)  $\alpha = \alpha(T, S, P)$  (5.12)

Determines the specific volume change of seawater as a function of state parameters:

$$d\alpha = \left(\frac{\partial \alpha}{\partial T}\right)_{SP} dT + \left(\frac{\partial \alpha}{\partial S}\right)_{TP} dS + \left(\frac{\partial \alpha}{\partial P}\right)_{TS} dP.$$
(5.13)

If you divide all the components of (1.37) by a particular unit volume  $\alpha_0$  the pre-fractions of temperature, salt and pressure will be:

- Thermal expansion coefficient:

 $K_{\rm T} = \frac{1}{\alpha_0} \left( \frac{\partial \alpha}{\partial \rm T} \right)_{\rm s.P}$ (5.14)

- Salt compression coefficient:

 $K_{\rm s} = -\frac{1}{\alpha_0} \left( \frac{\partial \alpha}{\partial S} \right)_{\rm T.P}$ 

- Compression resistance coefficient of density:

$$K_{\rm p} = -\frac{1}{\alpha_{\rm o}} \left( \frac{\partial \alpha}{\partial P} \right)_{\rm T.S}$$





Then the expression (5.14) is often called the equation of state in the differential form of seawater

$$\frac{d\alpha}{\alpha_0} = K_T dT - K_s dS - K_P dP$$
(5.15)

Currents theories often use simpler systems. The simplest of these is the Businesq approximation (the linear dependence of density on temperature):  $\frac{\rho}{\rho_0} = C_1 + C_2 \frac{T}{T_0} \qquad (5.16)$ 

and the linear dependence of density on temperature and salt (Linheikin, Robinson and Stommel, Bryan and Kox):

$$\frac{D}{D_0} = C_3 + C_4 \frac{T}{T_0} + C_5 \frac{S}{S_0}.$$
 (5.17)

Where T is temperature, S is salt,  $\rho_0$  is the average density of seawater; T<sub>0</sub> and S<sub>0</sub> are the average values of temperature and salt. When atmospheric pressure is equal 1 at, T<sub>0</sub>=17,5<sup>o</sup>C, S<sub>0</sub> = 35<sup>o</sup>/<sub>00</sub>,

 $\rho_0 = 1,02541 \text{ g/cm}^3 \text{ th}$  các hệ số có giá trị:  $C_1 = 1,00266$ ;  $C_2 = C_4 = -0,00317$ ;  $C_3 = 0,97529$ ;  $C_5 = 0,02737$ .

More precise dependence of density on temperature and salt:  $\frac{\rho}{\rho_0} = C_6 + C_7 \frac{T}{T_0} + C_8 \frac{S}{S_0} + C_9 \left(\frac{T}{T_0}\right)^2$  (5.18) with values T<sub>0</sub>, S<sub>0</sub>,  $\rho_0$  and atmospheric pressure as above C<sub>6</sub> = 0,97529, C<sub>7</sub>= - 0,00006, C<sub>8</sub> = 0,02737, C<sub>9</sub> = -0,0014.



If the compression of the liquid, i.e. the variation of density and the pressure ratio is taken into account, there

are:

$$\frac{\rho}{\rho_0} = \left[ C_6 + C_7 \frac{T}{T_0} + C_8 \frac{S}{S_0} + C_9 \left( \frac{T}{T_0} \right)^2 + C_{10} \frac{T}{T_0} \frac{S}{S_0} \right] \times \left[ 1 + \frac{P - P_0}{P_0} C_{11} \right]$$
(5.19)

Where  $P_0$  is pressure is equal to 1 at.,  $C_{11}$  is a constant quantity and a compression-resistant coefficient, can take:  $C_{10} = -0,00119$ ,  $C_{11} = 0,428.10^{-4}$ .

If you view the pressure as proportional to the depth, the equation (5.19) has:

$$\frac{\rho}{\rho_0} = \left[ C_6 + C_7 \frac{T}{T_0} + C_8 \frac{S}{S_0} + C_9 \left( \frac{T}{T_0} \right)^2 + C_{10} \frac{T}{T_0} \frac{S}{S_0} \right] \times \left[ 1 + C_{12} \frac{Z}{Z_0} \right]$$
(5.20)  
And simpler dependency(5.20) is: 
$$\frac{\rho}{\rho_0} = \left[ C_6 + C_7 \frac{T}{T_0} + C_8 \frac{S}{S_0} + C_9 \left( \frac{T}{T_0} \right)^2 + C_{10} \frac{T}{T_0} \frac{S}{S_0} \right] + C_{13} \frac{Z}{Z_0}$$
(5.21)

Where Z0 = 1km, it is possible to take C12 = 0.00428, C13 = 0.0043; (1.44) and (1.45) by Linheikin, Mamaev, Vaxilev. Equations (5.19) and (5.20), although not allowing for accurate calculation of density, have been used to solve most of the problems of sea current theory that involve examining the nonlinear interactions of the fields of flow velocity, density, temperature, and salt level.



The system of moving equations, continuous, state and preservation of salt heat is closed. But to get accurate results from solving those equations is impossible because the movement of the real liquid always has a tangled feature. Therefore, we must consider the tangled characteristics in these equations. Performs real motion in the form of medium motion and sublimation motion:

$$u = \overline{u} + u'; v = \overline{v} + v'; w = \overline{w} + w'$$

$$\mathbf{P} = \bar{P} + \mathbf{P}'; \mathbf{T} = \bar{T} + \mathbf{T}'; \mathbf{s} = \bar{s} + \mathbf{s}'; \rho = \bar{\rho} + \rho$$

MARE





#### **MOTION EQUATION IN TURBULENT MOTION**

At any time and points, the speed components must satisfy the Navie-Stoc equation, so according to the Ox axis we have:

$$\frac{\partial \bar{u}}{\partial t} + \frac{\partial u'}{\partial t} + (\bar{u} + u') \left(\frac{\partial \bar{u}}{\partial x} + \frac{\partial u'}{\partial x}\right) + (\bar{v} + v') \left(\frac{\partial \bar{u}}{\partial y} + \frac{\partial u'}{\partial y}\right) + (w' + \bar{w}) \left(\frac{\partial \bar{u}}{\partial z} + \frac{\partial u'}{\partial z}\right) = X - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x} - \frac{1}{\rho} \frac{\partial P'}{\partial x} + \upsilon \Delta \bar{u} + \upsilon \Delta \bar{u}'$$
(5.32)  
According to the Reynolds systems and the consequences we have:  

$$\bar{u'} = 0; \quad \frac{\partial \bar{u'}}{\partial x} = 0; \quad \frac{\partial \bar{u'}}{\partial t} = 0$$
(5.33)  
When we take the equation average (5.32) over the T period, we have:  

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \bar{w} \frac{\partial \bar{u}}{\partial z} + \frac{1}{u'} \frac{\partial u'}{\partial x} + \overline{v'} \frac{\partial u'}{\partial y} + \overline{w'} \frac{\partial u'}{\partial z} = X - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x} + \upsilon \Delta \bar{u}$$
(5.34)  
Hay:  

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \bar{w} \frac{\partial \bar{u}}{\partial z} = X - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x} - v \Delta \bar{u} - \frac{\overline{u'} \partial u'}{\partial x} - \frac{\overline{v'} \hat{u'}}{\partial y} - \frac{\overline{w'} \partial u'}{\partial z}} = X - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x} + v \Delta \bar{u} - \frac{\overline{u'} v'}{\partial y} - \frac{\partial u' v'}{\partial y} + u' \frac{\partial u'}{\partial x} + u' \frac{\partial v}{\partial y} + u' \frac{\partial v}{\partial z} = X - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x} + v \Delta \bar{u} - \frac{\overline{u'} v'}{\partial x} - \frac{\partial u' v'}{\partial y} - \frac{\partial u' w'}{\partial z} + u' \frac{\partial u'}{\partial x} + u' \frac{\partial u'}{\partial x} + u' \frac{\partial v'}{\partial y} + u' \frac{\partial v}{\partial z} = X - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x} + v \Delta \bar{u} - \frac{\overline{u'} v'}{\partial y} - \frac{\partial u' v'}{\partial y} - \frac{\partial u' w'}{\partial z} + u' \frac{\partial u'}{\partial x} + u' \frac{\partial v'}{\partial x} + u' \frac{\partial v'}{\partial x} + u' \frac{\partial v'}{\partial y} + u' \frac{\partial v'}{\partial y} + u' \frac{\partial v'}{\partial z} = X - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x} + v \Delta \bar{u} - \frac{u' v'}{\partial x} - \frac{\partial u' v'}{\partial y} - \frac{\partial u' w'}{\partial z} + u' \frac{\partial u'}{\partial x} + u' \frac{\partial v'}{\partial x} + u' \frac{\partial v'$$

When using continuous equations for medium and pulse motion and viewing the liquid as uncompressed, we

have:

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = \frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \frac{\partial \bar{w}'}{\partial z} = 0$$

Therefore:  $\frac{\partial \overline{u}}{\partial t} + \overline{u} \frac{\partial \overline{u}}{\partial x} + \overline{v} \frac{\partial \overline{u}}{\partial y} + \overline{w} \frac{\partial \overline{u}}{\partial z} = X - \frac{1}{\rho} \frac{\partial \overline{P}}{\partial x} = \upsilon \Delta \overline{u} - \frac{\overline{\partial u' v'}}{\partial x} - \frac{\overline{\partial u' v'}}{\partial y} - \frac{\overline{\partial u' w'}}{\partial z}$  $X - \frac{1}{\rho} \frac{\partial \overline{P}}{\partial x} + \frac{1}{\rho} \left( \varepsilon \Delta \overline{u} - \rho \frac{\overline{\partial u' z}}{\partial x} - \rho \frac{\overline{\partial u' v'}}{\partial y} - \rho \frac{\overline{\partial u' w'}}{\partial z} \right)$ 





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### **MOTION EQUATION IN TURBULENT MOTION**

Thus the Navie-Stoc equation with tangled motion has been taken on average different from the

previous equation of having additional nonlinear components.:

$\overline{\partial(\mathbf{u'}^2)}$	$\overline{\partial(\mathbf{u'v'})}$	$\overline{\partial(\mathbf{u'w'})}$
∂x	ду	∂z
$\partial(\mathbf{u'v'})$	$\overline{\partial(\mathbf{v'}^2)}$	$\partial(\mathbf{u'w'})$
∂x	∂y	∂z
$\overline{\partial(u'w')}$	$\overline{\partial(v'w')}$	$\overline{\partial(w'^2)}$
$\frac{\partial x}{\partial x}$	$\partial y$	$\partial z$

theo trục Ox;

theo trục Oy;

theo trục Oz;







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#### **Motion Equation In Turbulent Motion**

Similar to the viscous case of the element viscosity we have:

$$-\overline{\rho u'^{2}} = 2\varepsilon \frac{\partial \overline{u}}{\partial x} = \tau_{xx}$$

$$-\overline{\rho u'v'} = \overline{\rho v'u'} = \varepsilon \left(\frac{\partial \overline{v}}{\partial x} + \frac{\partial \overline{u}}{\partial y}\right) = \tau_{yx} = \tau_{xy}$$

$$-\overline{\rho u'w'} = \overline{\rho w'u'} = \varepsilon \left(\frac{\partial \overline{u}}{\partial z} + \frac{\partial \overline{w}}{\partial x}\right) = \tau_{zx} = \tau_{xz}$$

$$(5.36)$$

$$-\overline{\rho v'^{2}} = 2\varepsilon \frac{\partial \overline{v}}{\partial y} = \tau_{yy}$$

$$-\overline{\rho v'w'} = \overline{\rho w'v'} = \varepsilon \left(\frac{\partial v}{\partial z} + \frac{\partial \overline{w}}{\partial y}\right) = \tau_{zy} = \tau_{yz}$$

$$-\overline{\rho w'^{2}} = 2\varepsilon \frac{\partial \overline{w}}{\partial z} = \tau_{zz}$$

It is the component of reynolds tenxo or tangled tenxo of tangled motion:

$$\begin{pmatrix} \tau_{xx} & \tau_{yx} & \tau_{zx} \\ \tau_{xy} & \tau_{yy} & \tau_{zy} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{pmatrix}$$





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### Motion equation in turbulent motion

If you consider flat movement, the movement is constant.  $\frac{du}{dt} = 0$  have a speed (u) parallel to the Ox axis and depend only on z, there are:

$$0 = X - \frac{1}{\rho} \frac{\partial \overline{P}}{\partial x} + \frac{1}{\partial} \left( \varepsilon \frac{d^2 \overline{u}}{\partial z^2} - \rho \frac{du'w'}{dz} \right)$$
  
$$0 = X - \frac{1}{\rho} \frac{\partial \overline{P}}{\partial x} + \frac{1}{\partial} \frac{d}{dz} \left( \varepsilon \frac{d\overline{u}}{\partial z} - \rho \overline{u}'w' \right)$$
(5.37)

Similar to element friction, to find the turbulent viscosity coefficient  $\mu$  we write the pressure in the form of:  $F = \mu \frac{d\overline{u}}{dZ} = \varepsilon \frac{d\overline{u}}{dz} - \rho \overline{u'w'}$ 

Because in turbulent motion.  $\varepsilon \frac{d\overline{u}}{dz}$  very small compared to  $\rho \overline{u'w'}$  So we can skip and watch closely:  $F = \mu \frac{d\overline{u}}{dz} = -\rho \overline{u'w'}$ Therefore  $\mu = -\rho \frac{\overline{u'w'}}{\left(\frac{d\overline{u}}{d}\right)}$  (5.38)

It's a formula for calculating a turbulent viscosity coefficient. Theo Businesq the coefficient µ It depends mainly on the intensity of the disorder. The turbulent viscosity coefficient has a range from 101 - 103 CGS.



### Motion equation in turbulent motion

The assertion of u'v', u'w', v'w' in the other mean line does not allow to say that there must be some correlation between the ascension u', v', w'. When there is no correlation, u'v' is Zero. The correlation  $K = \frac{\overline{u'v'}}{\sqrt{\overline{u'^2}} \sqrt{\overline{u'^2}}}$ coefficient is calculated as follows: (5.39)

It has been determined that when the density is highly stable, the slime coefficient is small. So when the water mass has great stability, the Reynolds stress contains the w' component that must be smaller than reynolds stress without w', so the horizontal and vertical viscosity coefficients are different.

 $\tau_{\rm xz} = \tau_{\rm zx} = \mu_{\rm h} \frac{\partial \overline{\rm u}}{\partial z} + \mu_{\rm V} = -\rho \overline{{\rm u}' {\rm v}'}$  $\tau_{\rm xx} = 2\mu_{\rm V}\frac{\partial \bar{\rm u}}{\partial {\rm x}} = -\rho \overline{{\rm u}'^2} \qquad \qquad \tau_{zz} = 2\mu_{\rm h}\frac{\partial \bar{\rm w}}{\partial z} = -\rho \overline{{\rm w}'^2}$  $\tau_{yy} = 2\mu_{\rm V}\frac{\partial\bar{\rm v}}{\partial y} = -\rho\overline{{\rm v}'^2} \qquad \tau_{xy} = \tau_{yx} = \mu_{\rm V}\left(\frac{\partial\bar{\rm v}}{\partial x} + \frac{\partial\bar{\rm u}}{\partial y}\right) = -\rho\overline{{\rm u}'{\rm v}'} \qquad \tau_{xy} = \tau_{yx} = \mu_{\rm V}\left(\frac{\partial\bar{\rm v}}{\partial x} + \frac{\partial\bar{\rm u}}{\partial y}\right) = -\rho\overline{{\rm u}'{\rm v}'} \qquad (5.40)$ 

-  $\mu_{h}$  the turbulent viscosity coefficient of the horizontal speed gradient

-  $\mu_{\nu}$  the turbulent viscosity coefficient of the vertical speed gradient.




#### Motion equation in turbulent motion

If the pressure pressures act on a fluid volume factor.  $\delta x$ ,  $\delta y$ ,  $\delta z$ , with hypothesis  $\mu_h$  và  $\mu_v$  is constant and considering the continuity equation for average motion, there are:

$$\delta x \delta y \delta z \left( \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) = \delta x \delta y \delta z \left( \mu_h \frac{\delta^2 \bar{u}}{\partial x^2} + \mu_h \frac{\partial^2 \bar{u}}{\partial y^2} + \mu_h \frac{\partial^2 \bar{u}}{\partial z^2} \right)$$

The average motion equation is rewritten as:

$$\frac{d\bar{u}}{dt} = \frac{\partial\bar{u}}{\partial t} + u\frac{\partial\bar{u}}{\partial x} + \bar{v}\frac{\partial\bar{u}}{\partial y} + \bar{w}\frac{\partial\bar{u}}{\partial z} = X - \frac{1}{\rho}\frac{\partial\bar{p}}{\partial x} + \frac{\mu_{v}}{\rho}\left(\frac{\partial^{2}\bar{u}}{\partial x^{2}} + \frac{\partial^{2}\bar{u}}{\partial y^{2}}\right) + \frac{\mu_{h}}{\rho}\frac{\partial^{2}\bar{u}}{\partial z^{2}}$$

$$\frac{d\bar{v}}{dt} = \frac{\partial\bar{v}}{\partial t} + \bar{u}\frac{\partial\bar{u}}{\partial x} + \bar{v}\frac{\partial\bar{v}}{\partial x} + \bar{w}\frac{\partial\bar{v}}{\partial z} = Y - \frac{1}{\rho}\frac{\partial\bar{p}}{\partial y} + \frac{\mu_{v}}{\rho}\left(\frac{\partial^{2}\bar{v}}{\partial x^{2}} + \frac{\partial^{2}\bar{v}}{\partial y^{2}}\right) + \frac{\mu_{h}}{\rho}\frac{\partial^{2}\bar{v}}{\partial z^{2}}$$

$$\frac{d\bar{w}}{dt} = \frac{\partial\bar{w}}{\partial t} + \bar{u}\frac{\partial\bar{w}}{\partial x} + \bar{v}\frac{\partial\bar{w}}{\partial y} + \bar{w}\frac{\partial\bar{w}}{\partial z} = X - \frac{1}{\rho}\frac{\partial\bar{p}}{\partial z} + \frac{\mu_{v}}{\rho}\left(\frac{\partial^{2}\bar{w}}{\partial x^{2}} + \frac{\partial^{2}\bar{w}}{\partial y^{2}}\right) + \frac{\mu_{h}}{\rho}\frac{\partial^{2}\bar{w}}{\partial z^{2}})$$
(5.41)

Coefficients  $\mu_h \mu_v$  determined from Reynolds stress. Prandtl gives Reynolds stress formula as follows:

$$\tau_{zx} = -\rho \overline{\mu' w'} \left| \frac{d\overline{u}}{dz} \right| \frac{d\overline{u}}{dz}$$
(5.42) L is a turbulent road and  $\mu = \rho \ell^2 \frac{d\overline{u}}{dz}$ (5.43)

Thus the coefficient of  $\mu$  proportional to the cube of the turbulent distance.



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## Salt Conservation Equation in turbulent motion

We have:

$$\left[\frac{\partial}{\partial t} + (\bar{u} + u')\frac{\partial}{\partial x} + (\bar{v} + v')\frac{\partial}{\partial y} + (\bar{w} + w')\frac{\partial}{\partial t}\right](\bar{S} + S') = 0$$
(5.44)

If the liquid to be uncompressed,:

$$\frac{\partial \mathbf{u}'}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}'}{\partial \mathbf{y}} + \frac{\partial \mathbf{w}'}{\partial \mathbf{z}} = \mathbf{0}$$

And take the average equation (5.44) we have:  $\left(\frac{\partial}{\partial t} + \bar{u}\frac{\partial}{\partial x} + \bar{v}\frac{\partial}{\partial t} + \bar{w}\frac{\partial}{\partial t}\right)S + \frac{\partial}{\partial x}\overline{u'S'} + \frac{\partial}{\partial u}\overline{v'S'} + \frac{\partial}{\partial z}\overline{w'S'} = 0$  (5.45)

In the concept of a turbulent diffusion coefficient: Ax, Ay, Az of salt in the directions Ox, Oy, Oz. These coefficients are calculated according to expressions:  $\overline{u's'} = -\frac{A_x}{\rho}\frac{\partial\overline{s}}{\partial x}; \overline{v's'} = -\frac{A_y}{\rho}\frac{\partial\overline{s}}{\partial y}; \overline{w's'} = -\frac{A_z}{\rho}\frac{\partial\overline{s}}{\partial z}$  (5.46 Hence,  $\frac{\partial s}{\partial t} + \overline{u}\frac{\partial s}{\partial x} + \overline{v}\frac{\partial s}{\partial y} + \overline{w}\frac{\partial s}{\partial z} = \frac{\partial}{\partial x}\left(\frac{A_x}{\rho}\frac{\partial s}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{A_y}{\rho}\frac{\partial s}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{A_z}{\rho}\frac{\partial s}{\partial z}\right)$  (5.47)

(5.47) is the equation that diffuses salt in the sea. Similarly, we also found a thermal diffusion equation.  $\frac{\partial \overline{T}}{\partial t} + \overline{u} \frac{\partial \overline{T}}{\partial x} + \overline{v} \frac{\partial \overline{T}}{\partial y} + \overline{w} \frac{\partial \overline{T}}{\partial z} = \frac{\partial}{\partial x} \left( \frac{A_{Tx}}{\rho} \frac{\partial \overline{T}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{A_{Ty}}{\rho} \frac{\partial \overline{T}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{A_{Tz}}{\rho} \frac{\partial \overline{T}}{\partial z} \right)$ (5.48)





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## **BOUNDARY CONDITIONS**

Equations of motion are differential equations, in order to solve those equations, there must be boundary conditions or limit conditions. Boundary conditions are generally divided into three categories:

- **1.** Dynamic boundary conditions.
- 2. Kinetic boundary conditions.
- 3. Thermal and salt conditions.





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## **Dynamic boundary conditions**

These are conditions that indicate the continuity of the stressor at the boundary between the atmosphere and the ocean.

When  $z = -\zeta (x,y,t)$ , That is, on the free side of the ocean.:

Where Pa is the atmospheric pressure  $P = P_a$  (5.49)

$$\mu_{\rm h} \frac{\partial u}{\partial z} = -\tau_{\rm x}; \ \mu_{\rm h} \frac{\partial v}{\partial z} = -\tau_{\rm y}$$
(5.50)

where as TX, TY is a wind tangential stress on the sea surface.

Because of the lowering of ocean levels  $\zeta$  It is usually very small compared to the depth of the sea, so these conditions are sometimes given on the non-noisy side of the sea.: z = 0.







#### **Thermal and salt conditions**

These conditions denote the effect of the transport of thermal and salt through the dividing sides.

On the free side of the ocean.: Khi z = -  $\zeta(x,y,t)$  the general form of these conditions is:

$$\gamma T + \delta \frac{\partial T}{\partial z} = G_T \qquad \gamma S + \delta \frac{\partial S}{\partial z} = G_S \qquad (5.56)$$

if  $\delta = 0$  The condition is for the values of the function itself., and if  $\gamma = 0$  then for the gradient of that function.

- At the bottom and at the lateral solid boundaries, for conditions without the flow of thermal and salt according to the route method with the margin:  $\frac{\partial T}{\partial n} = \frac{\partial S}{\partial n} = 0$  (5.57)
- At the side fluids boundaries:  $\frac{\partial T}{\partial n} = G_{Tn}; \frac{\partial S}{\partial n} = G_{Sn}$  (5.58)

The initial conditions reflect the thermal state of the ocean at the initial time t = 0. It is usually required to give in advance the field of ocean features at the initial time:

$$u = u^{(0)}, v = v^{(0)}, w = w^{(0)}, p = p^{(0)}, T = T^{(0)}, s = s^{(0)}, \rho = \rho^{(0)}$$



# Classification of non-stop processes in the ocean and some approximations applied to currents research

When studying the ocean, there are seeing the phenomenon of fluctuations over time of marine fields such as the velocity field., temperature field  $T^0$ , salt degree field  $S^0/_{00}$ , density p..., they make up a variety of physical processes in the ocean. To classify these processes in time and space, similar to the classification of changes in climate fields, one derives from the spectrum of the cycle, which divides them into seven time periods.





- 1. Small-scale phenomena: Cycles from a few seconds to tens of minutes.
- 2. Medium-scale phenomena: Cycles from a few hours to daily.
- 3. Syn scale change: Cycles a few days to months
- 4. Season fluctuations: Five-year cycles and larger.
- 5. Changes between years: I.e. changes consistent with the state of large seas and of the entire atmosphere from year to year.
- 6. Changes in the century: Cycles of several decades. It is the study of the connection between the ocean and changes in the century of climate. \
- 7. Changes between centuries: Cycles of hundreds of years and larger. It is the study of the connection between the ocean and the fluctuations between the centuries of climate.



For average movements, the following approximations are correct.:

- **1. QUASI-STATIC APPROXIMATION**
- 2. APPROX. BUSINESQ
- 3. APPROXIMATIONS TO THE CORIOLIS FORCE
- 4. GEOLOCATION SYSTE







The studies of medium and large-scale processes in the ocean (vertical scale H  $\approx$  100 m ÷ 1 km and horizontal scale (L  $\approx$  100 ÷ 1000 km) show that vertical velocity is much smaller than horizontal velocity. Consider the order of quantity in the conservation of mass equation (the continuity equation): W = H.U/L suy ra W = 10<sup>-3</sup>U (5.60)

Where W, U are the characteristic quantities of the vertical and horizontal speeds.

Since the vertical velocity in the ocean is very small, it is possible to write the equation of vertical

motion as 
$$\frac{\partial P}{\partial z} = g \cdot \rho$$
 (5.61)

like the static equation.







We know that the density of water in the ocean changes very little :  $\frac{\partial \rho}{\rho} \approx 10^{-3} (\delta \rho \text{ is the})$ density anomaly), so density  $\rho$  can be replaced by  $\rho_0$  (average density), then the  $\overrightarrow{\text{divV}} = 0$ equation for conservation of mass is written as: (5.62)

(incompressible condition of seawater).





When studying medium- and large-scale motion in the ocean as known /W/ <</U/, the term with coefficient  $2\omega$ wcos $\phi$  in the component of the Coriolis force along the Ox axis can be ignored. But it may be necessary to account for this term in the narrow band at the equator.



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## **LECTURE**

## **MODELLING THE MARINE ENVIRONMENT**

## Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le







## Lecture 6

## **THEORY OF CURRENTS**

Lecturer: Professor. Nguyen Ky Phung Ms. Dang Thi Thanh Le







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#### I. GEOSPHERE CURRENTS

- 1. Inclination of isobaric surface
- 2. Method of dynamic calculation of geosphere currents

### **II. STEADY CURRENTS THEORY**

- 1. Ekman's theory with deep currents
- 2. Ekman's theory for the shallow sea
- 3. The development of fluency currents
- **III. GRADIENT CURRENTS THEORY**







#### **\* INCLINATION OF ISOBARIC SURFACES IN FLUIDS**

In the conditions that (1) frictionless horizontal flow at a constant speed, (2) the single external force (gravity), and (3) no vertical movement, the horizontal components of Coriolis force and gradient pressure are balanced:

$$2\omega \sin \varphi \, v = \frac{1}{\rho} \frac{\partial P}{\partial x}$$

$$2\omega \sin \varphi \, u = -\frac{1}{\rho} \frac{\partial P}{\partial y}.$$
(6.1)

If we take the cubes of each equation and add them together, we have:

$$\frac{\partial P}{\partial n} = 2\omega\rho c \sin\varphi \qquad (6.2)$$

$$\dot{O} \, d\hat{a}y \quad c = (u^2 + v^2)^{1/2}, \\ \frac{\partial P}{\partial n} = \left[ \left( \frac{\partial P}{\partial x} \right)^2 + \left( \frac{\partial P}{\partial y} \right)^2 \right]^{1/2}$$







#### **\* INCLINATION OF ISOBARIC SURFACES**

Equation (6.2) shows the requirement for the forces balance is the equalization between the Coriolis force and horizontal pressure. Thus, the horizontal flow vector is parallel to the broken isobaric lines in a direction that the larger isobaric lines in the Northern Hemisphere have located on the right in the direction of the flow and vice versa in the Southern Hemisphere. This type of flow is called the *barotropic flow* and the balance of forces represented by equation (6.2) is called the *barotropic flow* equilibrium.







#### **\* INCLINATION OF ISOBARIC SURFACES IN FLUIDS**

Replace the horizontal pressure gradient in Equation (6.1) with the angle of inclination of the isobaric surfaces. Figure 6.1a shows the inclination of the isostatic surfaces relative to the equipotential surfaces. The nOz plane is perpendicular to the flow rate c. Pressure at point A is equal to "P" and at point B is equal to " $P + \Delta P = P + \rho g \Delta z$ ", where  $\rho$  – water column density between points C and *B* 



Figure 6.1. Inclination of isobaric surfaces







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#### Inclination OF ISOBARIC SURFACES

Thus:

$$\frac{\Delta P}{\Delta n} = \rho g \frac{\Delta z}{\Delta n}$$

$$\frac{\partial P}{\partial n} = \rho g t g \beta$$
(6.3)

If the Oz axis trend downwards, the angle  $\beta$  will follow clockwise rotation. From equations (6.2) and (6.3), the tg values  $\beta$  express as:

$$\operatorname{tg}\beta = \frac{2\omega c\sin\varphi}{g}$$

From those equations, the angle of inclination of an isobaric surface is proportional to the flow rate at the depth of that surface.







#### **\* INCLINATION OF ISOBARIC SURFACES**

The impact of the Coriolis force in actual currents creates the horizontal Circulation trend. As a result, lighter water in the upper layer moves on the right side of the flow direction and vice versa while the Southern Hemisphere sees the opposite movement. Therefore, with the same inclination of isobaric surfaces, the inclination of isopycnic surfaces appears. The angle between isobaric surfaces and isobaric volume is contrary. Moreover, the inclination of isopycnic surfaces appears somehow leads to the inclination of isobaric surfaces which causes horizontal gradient pressure. The distribution of isopycnic surfaces can relate to the water movement,







#### ✤ INCLINATION OF ISOBARIC SURFACES IN FLUIDS

 $b_1b_2 = b_1n + b_2n$ 

Figure 6.1b shows the inclination of the isopycnic curves relative to the isostatic surfaces. Since the pressures  $q\rho_1(b_1b_2) = q\rho_2(a_1a_2)$ (6.5)at points a2 and b2 are equal, then: :

Besides,

$$a_1a_2 = a_1m + a_2m \qquad \qquad h m$$

$$b_1 b_2 = b_1 n + b_2 n$$

$$a_1 a_2 = a_1 m + a_2 m$$

$$\frac{b_1 n}{a_1 n} = tg \beta_1$$

$$\frac{a_2 m}{b_2 m} = tg \beta_2$$

$$\frac{b_2 n}{a_1 n} = tg \gamma$$

(6.6)Ta change of expression (6.5), simplified  $g: \rho_1(a_1 n \lg \beta_1 + a_1 n \lg \gamma) = \rho_2(a_1 n \lg \gamma + a_1 n \lg \beta_2)$ 

simplified the number of term  $a_1 n$  and substitute (6.6) the values:  $t g \beta_1 = \frac{2\omega c_1 \sin \varphi}{\alpha}$  và  $t g \beta_2 = \frac{2\omega c_2 \sin \varphi}{\alpha}$ 

$$\operatorname{tg} \gamma = \frac{2\omega \sin \varphi}{g} \cdot \frac{\rho_1 c_1 - \rho_2 c_2}{\rho_2 - \rho_1}$$







#### **\* INCLINATION OF ISOBARIC SURFACES IN FLUIDS**

In meteorology, this similar to the Margules formula which is:

- 1) The position of the isopycnic lines on the cross-section allows consideration of the presence of flow perpendicular to the plane of the section and its direction;
- 2) The greater the inclination of the isopycnic lines, the smaller the density difference of the layers, the larger the speed difference. In immobilized layers, the isopycnic curves as well as the isobaric lines are horizontal
- 3) If layers of the same density move at different velocities, then  $\gamma = 90^{\circ}$ . In this case, the layers are very unstable and the  $\gamma$  has no meaning.







#### **\* METHOD OF DYNAMIC CALCULATION OF GEOSPHERE CURRENTS**

From the equations (6.1), find equation for u and v:

$$u = -\frac{1}{2\omega\rho\sin\varphi} \cdot \frac{\partial P}{\partial y} = -\frac{\alpha}{2\omega\sin\varphi} \cdot \frac{\partial P}{\partial y}$$
$$v = \frac{1}{2\omega\rho\sin\varphi} \cdot \frac{\partial P}{\partial x} = \frac{\alpha}{2\omega\sin\varphi} \cdot \frac{\partial P}{\partial x}$$
(6.8)

These equations represent the balance between the horizontal composition of the friction force and the Coriolis force produced by the movement itself.

Because:  $\alpha \partial P = \partial D$ , then the expressions (6.8) can be rewritten as follows:  $U = \frac{1}{2\omega \sin \varphi} \cdot \frac{\partial D}{\partial y} V = \frac{1}{2\omega \sin \varphi} \cdot \frac{\partial D}{\partial x}$  (6.9) If the direction of n is the greatest inclination of the isotropic side, then we have the speed:  $c = \frac{1}{2\omega \sin \varphi} \cdot \frac{\partial D}{\partial n}$  (6.10) Where  $\frac{\partial D}{\partial n}$  actual inclination of the isobaric surfaces relative to the equipotential plane





#### **\* METHOD OF DYNAMIC CALCULATION OF GEOSPHERE CURRENTS**

The relative "inclination" between two hydrological stations is not difficult to determine. Suppose we have two hydrological stations A and B. Consider two isostatic surfaces  $P_1$  and  $P_2$ . Let the distance between A and B be  $\ell$ . Then, for the isobaric surface P1, the flow rate in the direction perpendicular to AB is :

$$C_1 = \frac{D_{B_1} - D_{A_1}}{2\omega\ell\sin\varphi}$$

The line segment  $AB = \ell$  is accepted as the differential factor dn , dynamic height  $D_{A_1}$  and  $D_{B_1}$  of the isobaric surface P1 relative to the equipotential surface is unknown at present. The speed at the isobaric surface P2 is determined by the same formula:  $C_2 = \frac{D_{B_1} - D_{B_2}}{2\omega\ell\sin\omega}$ 

Take the first expression minus the second, we have results as below

$$C_1 - C_2 = \frac{\left(D_{B_1} - D_{B_2}\right) - \left(D_{A_1} - D_{A_2}\right)}{2\omega\ell\sin\varphi} = \frac{\Delta D_B - \Delta D_A}{2\omega\ell\sin\varphi}$$

(6.11)







#### **\* METHOD OF DYNAMIC CALCULATION OF GEOSPHERE CURRENTS**

Thus, the dynamic method only allows for determining the difference in speeds. If we know the flow rate at a certain cross-section (where the flow velocity is zero), the problem is simply solved. But in practice, we almost always do not know that speed, so the problem is how to choose the zero surface. Thanks to equation (6.11), it is possible to calculate the real speed of the flow at different water levels.

Based on equation (6.10), it can be determined that the zero surface is the depth at which the horizontal gradient components of the dynamic depth approach 0.







#### **\* METHOD OF DYNAMIC CALCULATION OF GEOSPHERE CURRENTS**

The Defant method is the most common method for choosing the zero side, which is based entirely on the dynamic characteristics of the flow and does not contain assumptions like other methods.







#### **\* METHOD OF DYNAMIC CALCULATION OF GEOSPHERE CURRENTS**

When searching for zero surfaces, Defant noticed that most of the differences in curves between dynamic depths in two oceanographic stations (Figure 6.2) for different station pairs are characterized by the existence of more or less straight segments. standing, for pairs of neighboring stations, they are distributed at approximately the same depths.

Within those segments, the dynamic depth differences remain constant. This means the speeds of the currents are identical.

If the 0 mark is not located in the vicinity of this vertical segment, then in the whole layers that have no difference in flow rates. If the 0 mark is not located far enough from this section, then the flow rates in the entire layer will be equally large. The latter is also less realistic, so Defant assumes that the flow rates throughout the layer are equal to the difference between the same dynamic depths, while the zero surface is in the center of the layer.





#### **\* METHOD OF DYNAMIC CALCULATION OF GEOSPHERE CURRENTS**

There is another method is use to select the zero surface based on the analysis of the individual volume difference curves between neighbouring stations – Parr's method. This method is attributed to the identification of variations in water layers between selected mass isomorphs and so on.

Since the fact that in the World Ocean does not exist on a single (continuous) side, instead of using a reference side as common, the geosphere currents are assumed to equal zero. For this purpose, the reference surface chosen in the class between 1000 and 2000 m is quite appropriate, while the surface at 3000 m of depth is chosen in some examples such as the southern Ocean







#### **\* METHOD OF DYNAMIC CALCULATION OF GEOSPHERE CURRENTS**

Other difficulties in determining the zero side, the method of dynamic calculation also has a series of disadvantages:

- As not mention to the pure flow component under the direct impact of tangential wind stress, exclusive the speed and direction of the wind, the swirling and non-stop components caused by forces not present in the basic equation (6.11), as well as ignoring the seabed topography.
- In addition, large deviations in flow rate can appear if the hydrological cross section is stimulated for a long period of time, furthermore not perpendicular to the direction of the flow, the distance between stations is not the same and quite large, especially in areas with front.







#### **\* METHOD OF DYNAMIC CALCULATION OF GEOSPHERE CURRENTS**

Despite such major drawbacks, the method of dynamic calculation due to simplicity and ease of use has been recognized worldwide and remains valid to this day. This method is often applied to standard cross sections, when performing standard cross sections always have to compare the results received with the estimated data in previous years. We also note that ocean circulation maps built on dynamic methods (Shott, 1933, Sverdrup, 1941, Ditrich, 1961, etc.) are generally quite consistent with observational data and overall ocean circulation mathematical modeling results.







#### **\* DYNAMIC METHODS FOR CALCULATION OF GEOGRAPHIC FLUID**

Figure 6.3 shows the dynamic surface

map of Nam Duong as an example.

Figure 6.3: The dynamic surface map of

Nam Duong as an example





## **THEORY OF CURRENTS**

MARE







#### Ekman theory with deep currents

Since the friction stress of the wind is greater than the other forces that cause the flow, on average the wind flow contributes the largest part to the total speed of the flows, especially in the upper layer of the ocean. Ekman made the following assumptions:

- 1. The sea is shoreless and infinitely deep (to eliminate the effect of friction with the shore and bottom);
- 2. Wind and currents caused by it are stable and do not change over time;
- 3. The wind and current speed fields do not vary in the horizontal direction (no divergence);
- 4. The vertical component of the speed is absent because the motion occurs only in the horizontal direction and does not diverge;
- 5. Sea is homogeneous in density (to exclude density flow) and incompressible water;
- 6. The sea surface is the horizontal plane (to exclude the gradient component);
- 7. The accepted coefficient of tangle friction  $A_z$  remains constant with depth







#### Ekman theory with deep currents

With all the assumptions for steady flow, a turbulent frictional is the only force that transmits the impact of wind stress down to the depth and the Coriolis force is equal to it. The equation of motion in this case has the form: Here we put:

$$\frac{A_z}{\rho} \frac{d^2 u}{dz^2} + 2\omega v \sin \varphi = 0$$
$$\frac{A_z}{\rho} \frac{d^2 v}{dz^2} - 2\omega u \sin \varphi = 0$$

Transform the expressions above into forms:

$$\frac{d^2u}{dz^2} + \frac{2\rho}{A_z}\omega v\sin\varphi = 0$$
(6.12)  

$$\frac{d^2v}{dz^2} - \frac{2\rho}{A_z}\omega u\sin\varphi = 0$$
ns (6.12) are rewritten to: 
$$\frac{d^2u}{dz^2} + 2a^2v = 0$$
(6.12)

 $\frac{d^2v}{dz^2}$ 

 $-2a^2u=0$ 

- The Y axis to coincide with the wind direction,

- The X axis is towards the right,

- The 7 axis is pointing down

If symbolize:  $\frac{\rho \omega \sin \varphi}{A_z} = a^2$  Then the equations (6.12) are rewritten to:





#### Ekman theory with deep currents

This is a system of second-order ordinary differential equations and solutions of the form :

 $u = c_1 e^{az} \cos(az + \phi_1) + c_2 e^{-az} \cos(az + \phi_2)$  $(c_1, c_2, \phi_1, \phi_2 - \text{ constants})$  $v = c_1 e^{az} \sin(az + \phi_1) - c_2 e^{-az} \sin(az + \phi_2)$ 

We state the first boundary condition: the flow rate when increasing depth needs to be limited, i.e.  $u \neq \infty, v \neq \infty$  khi  $Z \rightarrow \infty$ 

In this case, c1 must be zero, otherwise, the increasing of (z) the speed will increase infinitely. At the same time, it is no longer necessary to identify  $\phi_1$ .

We rewrite the equations (6.14) as follows:  $u = c_2 e^{-az} \cos(az + \phi_2)$ ;  $v = -c_2 e^{-az} \sin(az + \phi_2)$ (6.15)

We set out the second boundary condition:

At sea surface z = 0

Wind tangeriial stress

$$=A_{z}\frac{dc}{dz}$$

τ

 $-A_z \frac{du}{dz} = 0$ 

- And axis Y in the direction gió.

Then, at z = 0 and the edge stress in the water just below the ocean surface will be equal to the wind gland friction, we have:







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#### Ekman theory with deep currents

The speed module symbol at the surface is  $U_0$ , when:

$$U_0 = \sqrt{u^2 + v^2} = \frac{\tau}{\sqrt{2}A_z a}.$$
 (6.17)

Substituting the value to equation (6.17), we get

$$U_0 = \sqrt{u^2 + v^2} = \frac{\tau}{\sqrt{2}A_z a}.$$
 (6.18)

Equation (6.17) can draw the conclusion that with the same conditions, the flow velocity decreases as latitude increases. Along with (6.17) the equations (6.15) can be rewritten

$$u = U_0 e^{-az} \cos(45 - az)$$
  
 $v = U_0 e^{-az} \sin(45 - az)$ 
(6.19)




## **STEADY CURRENTS**



#### Ekman's theory with deep current



according to Ekman

Along with a decrease in speed with depth, the current turns to the right relative to its direction at sea level.

Figure 6.4 represents the speed line described in the shape of loga twist and represents a change in direction and the speed of wind flow in depth. Figure 6.4 shows that, at some depth, the speed vector will point in the opposite direction to the face flow.

It is often referred to as the depth of friction (rather the impact depth of friction) and the symbol in D.:

$$D = \frac{\pi}{a} = \pi \sqrt{\frac{A_z}{\rho \omega \sin \varphi}}$$





#### **STEADY CURRENTS**



#### Ekman theory with deep currents

The quantity Az is difficult to determine, so when there is flow monitoring data in the ocean surface layer, it is possible to find Az from formula (6.20) if the quantity D is known:

$$A_z = \frac{D^2 \rho \omega \sin \varphi}{\pi^2} \tag{6.21}$$

The total flux of the drift is determined by integrating from zero to infinity in the coordinate axes directions:

$$S_x = \int_0^\infty u dz \text{ và } S_y = \int_0^\infty v dz \qquad (6.22)$$

Substitute u and v from (6.19) to (6.22):

$$S_x = U_0 \int_0^\infty e^{-az} \cos(45^\circ - az) dz$$
  $S_y = U_0 \int_0^\infty e^{-az} \sin(45^\circ - az) dz$ 







#### Ekman's theory for the deep sea

$$\int e^{az} \sin b \, x \, dx = \frac{e^{az}}{a^2 + b^2} (a \sin b x - b \cos b x) \, , \, \int e^{az} \cos b \, x \, dx = \frac{e^{az}}{a^2 + b^2} (a \cos b x - b \sin b x)$$

$$S_x = \frac{U_0 e^{-az}}{2a^2} [-a \cos(45 - az) - a \sin(45 - az)] \Big|_0^\infty = \frac{U_0}{2a^2} a \sqrt{2} = \frac{U_0 \sqrt{2}}{2a}$$

$$= U_0 \sqrt{2}/2a \cdot \pi/a \cdot a/\pi = \frac{U_0 \sqrt{2}D}{2\pi}$$

$$S_y = \frac{U_0 e^{-az}}{2a^2} [-a \sin(45 - az) + a \cos(45 - az)] \Big|_0^\infty = 0$$

$$S_x = \frac{U_0 \sqrt{2}D}{2\pi}, \qquad S_y = 0$$







#### **STEADY CURRENTS**



#### **\*** Ekman's theory for the shallow sea

There is no difference in results for the shallow sea. By integral equation (6.13) and sets the additional conditions so that at the seabed both the speed components of u and v are equal to zero. Without repeating all of Ekman's arguments, we write:

 $u = Asha\xi \cos a \xi - Bcha\xi \sin a \xi$  $v = Acha\xi \sin a \xi + Bsha\xi \cos a \xi$ 

 $\xi$  - vertical coordinates at the base.

The constants analyzed by A and B are equal to:

$$A = \frac{\tau D}{\pi A_z} \frac{\operatorname{ch} a \operatorname{dcos} ad + \operatorname{sh} a \operatorname{dsin} ad}{\operatorname{ch} 2 \operatorname{ad} + \operatorname{cos} a \operatorname{d}}$$
$$B = \frac{\tau D}{\pi A_z} \frac{\operatorname{ch} a \operatorname{dcos} ad - \operatorname{sh} ad \operatorname{sin} ad}{\operatorname{ch} 2 \operatorname{ad} + \operatorname{cos} a \operatorname{d}}$$

With d - is sea depth





### **STEADY CURRENTS**



#### Ekman's theory for the shallow sea

The angle between the flow direction at the surface and axis Y is determined by the expression:

 $tg(U_0, Y) = \frac{U_0}{V_0} = \frac{s h 2ad - si n 2ad}{s h 2ad + si n 2ad}$ (6.25) where 2ad is the depth of sea  $2ad = 2ad \frac{\pi}{a} \frac{a}{\pi} = \frac{2\pi d}{D}$ 

Then the quantity d/D can be consider as shallow water indicator

The table below shows the  $\alpha$  value between the flow vector and the wind vector that depends on the quantity d/D

d/D	0.1	0.25	0.5	0.75	1	>1
α	5	21.5	45	45.5	45	45

From Figure 6.5 this infers that, when d > D the speed of the vectors the actual flow speed coincides with the case of the infinite deep sea (see Figure 6.4).



Figure 6.5 Current velocity heads in the sea of finite depth depending on the d/D ratio







#### The development of fluency currents

Before stabilizing, the direction and velocity of flow may be much different than defined by formulas

(6.19) and (6.24). Ekman looked at the development of drift currents in case the wind with constant

intensity and direction began to effect the silent sea surface in a stable state. There is seeing that the

flow at different water levels develops differently and the deeper you dive, the later stability appears.





#### **STEADY CURRENTS**



#### The development of flowing currents

In Figure 6.6, the endpoint of the unstable flow vector draws a complex spiral-shaped curve that gradually approaches a stable value.



Figure 6.6. The velocity curve shows the development of pure drift current at the sea surface (time from wind arrival is constant equal to pendulum hours).



### **GRADIENT CURRENTS THEORY**



In nature, the rise and fall of water surface occurs even far from shore. The inclination of the sea surface can create a pressure gradient that causes the gradient currents. Ekman made the following assumptions to simplify the process:

1) The landless sea and homogeneous in density;

2) The inclination of the sea surface is constant and stable in time and space;

3) Flat seabed;

- 4) Stable flow, no vertical components;
- 5) There is no fluctuation in the turbulent viscosity coefficient with depth.







In this case, the following impact forces are the horizontal pressure, the Coriolis force, and the friction force in which the bottom friction is transmitted vertically, which constrains movement.

Motion equations write in the form of:

$$\frac{A_z}{\rho}\frac{d^2u}{dz^2} + 2\omega\nu\sin\varphi = 0 \qquad \qquad \frac{A_z}{\rho}\frac{d^2\nu}{dz^2} - 2\omega\nu\sin\varphi + g\sin\beta = 0 \qquad (6.26)$$

Formulas for determining gradien flow rate components are written as:

$$u = \frac{g\sin\beta}{2\omega\sin\varphi} \left[ 1 - \frac{\operatorname{ch} a(H+z)\cos a(H-z) + \operatorname{ch} a(H-z)\cos(H+z)}{\operatorname{ch} 2aH + \cos 2aH} \right]$$
(6.27)  
$$v = \frac{g\sin\beta}{2\omega\sin\varphi} \left[ \frac{\operatorname{sh} a(H+z)\sin a(H-z) + \operatorname{sh} a(H-z)\sin(H+z)}{\operatorname{ch} 2aH + \cos 2aH} \right]$$



#### **GRADIENT CURRENTS THEORY**



Figure 6.7.

Based on equations (6.27), (Figure 6.7a), the construction of the first curve's velocity current for three values of sea depth is expressed as a fraction of the depth friction. Figure 6.7 shows the stereoscopic change of gradient flow in different depths.









## **GRADIENT CURRENTS THEORY**

At the seabed, the currents are zero according to the condition. As the increase in distance from the bottom, the flow velocity increases slowly turns to the right direction compared to the inclination of the water level. As the water depth large enough, maximum speed and deflection angle 90° achieved at a distance  $D = \frac{\pi}{a}$  from the bottom. Since continuing leave from the bottom, the speed and direction of the flow remain constant until reaching the surface. As such, the influence of bottom friction is spread upwards within the range layer of the D-thickness. Similar to the influence of the depth of friction in the Ekman drift, this layer is called the lower friction (the lower boundary of the depth influence the bottom friction).

The total gradient flux has components in both coordinate axes. The Y-axis composition is only significant in the layers near the bottom and when H > D it reaches a defined finite limit like the X-axis component:  $S_y \rightarrow \frac{Dg\sin\beta}{4\pi\omega\sin\varphi}, S_x \rightarrow \frac{g\sin\beta}{2\omega\sin\varphi} \left(H - \frac{D}{2\pi}\right)$ (6.28)



#### **LECTURE**

## **MODELLING THE MARINE ENVIRONMENT**

Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le







#### Lecture 7

#### **PROCESS OF SUBSTANCE TRANSMISSION**

Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le





#### Lecture 7A

#### **MASS BALANCING EQUATION**

Cán Bộ Giảng Dạy: GS.TS. Nguyễn Kỳ Phùng ThS. Đặng Thị Thanh Lê





## MASS balancing equation

## Steady - state system Solution

- Transfer functions
- Residence

## Unsteady - state system Solution

- Impulse loading
- Step loading
- Linear loading
- Exponential loading
- Sinusodial loading



A completely mixing system. (CSTR – Continuously Stirred Tank Reactor) It's the simplest system that can be used to model a real water body.



For a finite time period, the mass balance of the system is described by the equation:

Accumulation = Loading - OutFlow - Reaction - Settling

MASS BALANCE FOR A WELL-MIXED LAKE (Cont)

Accumulation: represent the change of Mass M of the system over a period of time t.

Accumulation 
$$= \frac{\Delta M}{\Delta t}$$
  
 $c = \frac{M}{V} \rightarrow M = Vc$ 
 $\rightarrow Accumulation = \frac{\Delta Vc}{\Delta t} [MT^{-1}]$ 

If V is constant

Accumulation = 
$$V \frac{\Delta c}{\Delta t} \rightarrow V \frac{dc}{dt}$$
  $\frac{dc}{dt} > 0 \rightarrow$  Increased accumulation  
 $\frac{dc}{dt} < 0 \rightarrow$  Reduced accumulation  
 $\frac{dc}{dt} = 0 \rightarrow$  Constant

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#### Loading :

 $c_{in}(t)$  : concentration[ML<sup>-3</sup>]

Point source (source identity, convenient measurement, continuality)

- + Municipal wastewater
- + Industrial wastewater
- + Tributary

#### Distribution source

- Agriculture
- Atmosphere
- Water flowing from the city.
- Groundwater



### ♦ Outflow:

**\*** A WELL-MIXED LAKE :  $c = c_{out}$ 

$$\rightarrow$$
 Outflow = Q $c_{out}$  = Q $c$ 

✤<u>Reaction:</u>

Reaction = kM = kVc

k: First order reaction coefficient [T<sup>-1</sup>]

\*Settling:

Settling = 
$$vA_sc$$
  
 $V = A_sH$   
 $\rightarrow$  Settling =  $\frac{v}{H}Vc = k_sVc$ 

*v*: apparent settling velocity[LT<sup>-1</sup>]

 $k_s$ : a first – oder settling rate constant= v/H [T<sup>-1</sup>] H: depth[L]







#### Mass balancing equation

$$W\frac{dc}{dt} = W(t) - Qc - kVc - vA_sc$$

- Dependent variable: c
- Independent variable : t
- Impact function: W(t), which represents external influence on the system
- Parameter: V, Q, k, v, và A<sub>s</sub>



Mass balance equation

$$V\frac{dc}{dt} = W(t) - Qc - kVc - vA_sc = 0$$

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

> Assimilation agent (self-cleansing ability)

$$a = Q + kV + vA_s$$



## Example 1:

A lake has the following characteristics: volume =  $50,000 \text{ m}^3$ , depth = 2m, inflow = outflow =  $7500\text{m}^3$ /day, temperature =  $25^{\circ}\text{C}$ . The lake receives the input of pollutants from three sources:

- a factory discharge of 50 kg/day
- a flux from the air with a load of 0.6 g/m<sup>2</sup>/day
- the inflow stream has a concentration of 10mg/l
- If the pollutant decay at the rate of 0.25/day at 20<sup>o</sup>C ( $\theta$ =1.05).
- a) Calculation of assimilation agents.
- b) Determine the steady state concentration

c) Calculates the mass per time for each term in the mass balance and displays your results on a plot.





#### \* Transter function

$$c = \frac{W}{Q + kV + vA_s} = \frac{Qc_{in}}{Q + kV + vA_s}$$
$$\rightarrow \frac{c}{c_{in}} = \beta = \frac{Q}{Q + kV + vA_s}$$
: Transfer function

- Transfer function : it specified how the system input is transformed into an output
- $\beta \ll 1$ : the mechanical cleaning of the lake will reduce the concentration of pollution (high assimilation capacity)
- $\beta \rightarrow 1$ : weak lake cleaning mechanics



## Residence time

The residence time of a substance E represents the mean amount of time that a particle of E would reside in a system.

$$\tau_{\rm E} = \frac{\rm E}{|\rm dE/\rm dt|_{\pm}}$$

E: Quantity of E in a specified volume [M or  $ML^{-3}$ ]

 $|dE/dt|_{\pm}$ : absolute value of source or lake [MT<sup>-1</sup>or ML<sup>-3</sup>T<sup>-1</sup>]

- The residence time of the water in the lake:  $\tau = \frac{V}{\Omega}$
- The residence time of pollutants in the lake

$$\tau = \frac{Vc}{Qc + kVc + vA_sc} = \frac{V}{Q + kV + vA_s}$$





### Example 2:

A lake has the following characteristics: volume =  $50,000 \text{ m}^3$ , depth = 2m, inflow = outflow =  $7500\text{m}^3/\text{day}$ , temperature =  $25^0\text{C}$ . The lake receives the input of pollutants from three sources:

- a factory discharge of 50 kg/day
- a flux from the air with a load of 0.6 g/m<sup>2</sup>/day
- the inflow stream has a concentration of 10mg/l

If the pollutant decay at the rate of 0.25/day at 20<sup>o</sup>C ( $\theta$ =1.05).

- a) Inflow concentration.
- b) Transfer function
- c) The residence time of the water
- d) The residence time of pollutants



**Exercises**: A lake has the following characteristics.:

Surface area =  $2x10^5$  m<sup>2</sup>, Medium depth = 3 m, Q in= Q out = 45000 m<sup>3</sup>/day, inflow BOD concentration = 4mg/l, residence time = 2 week

A subdivision housing 1 000 people will discharges raw sewage into this system. Individual contributes about

150 x 3.785 litter/day

and 0.25 x 453.6 g/day.

- a) Determine the BOD concentration of wastewater (mg/l).
- b) If BOD decay =  $0.1 \text{ day}^{-1}$  and settles at rate of 0.1 m/day. Calculate the assimilation factor for lake prior to building subdivision housing .
- c) Calculation of transfer function factor after subdivision housing.
- d) Determine the steady concentration of the lake in both cases with and without subdivision housing.

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At a certain point, if the reduction in pollutant emissions takes place, two questions will be asked as follows:

- How long will the water quality be restored?
- What is the "shape" of this recovery?

# UNSTEADY- SYSTEMS SOLUTION (CONT)

To determine the path of pollutants, consider the equation of mass balance:

$$V\frac{dc}{dt} = W(t) - Qc - kVc - vA_sc$$

$$\leftrightarrow \frac{dc}{dt} = \frac{W(t)}{V} - \frac{Q}{V}c - kc - \frac{v}{H}c$$

$$\leftrightarrow \frac{dc}{dt} + \lambda c = \frac{W(t)}{V} \qquad (*)$$
With  $\lambda = \frac{Q}{V} + k + \frac{v}{H}$ : eigenvalue

If Q, V, k, v, H is constant, equation (\*) are differential equations, first order, linear, and heterogeneous. The solution consists of two parts:

$$c = c_g + c_p$$

 $c_g$ : Generalized solution for the case W(t) = 0

 $c_p$ : particular solution for specified form W(t)

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## **\***General slolution(c<sub>g</sub>)

- W(t) = 0: c = c<sub>g</sub>
- At t =0: c = c<sub>0</sub>  $\rightarrow$  solution of equation (\*) is: c = c<sub>0</sub>e<sup>- $\lambda$ t</sup>







#### Response time

- The time the lake needs to recover..
- $t_{\phi}$  = **Response time**  $\phi$ %, which means the time it takes to achieve it.  $\phi$ % the final level of recovery of the lake..

$$t_{\phi} = \frac{1}{\lambda} \ln \frac{100}{100 - \phi}$$

Response time	t <sub>50</sub>	T <sub>63.2</sub>	t <sub>75</sub>	t <sub>90</sub>	t <sub>95</sub>	t <sub>99</sub>
Formula	0.693/λ	1/λ	1.39/λ	2.3/λ	3/λ	4.6/λ

## **WINSTEADY- SYSTEMS SOLUTION (CONT)**

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#### Example 3

For a lake has the following characteristics: volume  $=50,000m^3$ , depth = 2m, Inflow = outflow =  $7500m^3/day$ , temperature =  $25^{0}C$ , waste loading= 140,000g/day, Decay rate=  $0.319 d^{-1}$ 

- If the initial concentration is equal to a steady state level (5.97 mg/l), determine the general solution.
- Determine the response time 75%, 90%, 95%, and 99%

**NSTEADY- SYSTEMS SOLUTION (CONT)** 

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#### Particular solutions(c<sub>p</sub>): Loading function





Particular solutions: Integrating factor method.

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

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

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

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

$$\frac{dc}{dt} (e^{\lambda t} c) = e^{\lambda t} \frac{W(t)}{V}$$

$$c(t) = c_0 e^{-\lambda t} + \frac{e^{-\lambda t}}{V} \int e^{\lambda t} W(t) dt$$

Cg



Cn

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## UNSTEADY- SYSTEMS SOLUTION (CONT)



#### ✤ IMPULSE LOADING (SPLII)

Describes the discharge that takes place in a short time.

Impulse function:  $W(t) = m\delta(t)$  (m: quantity of pollutant mass[M])

Equation(\*): 
$$\frac{dc}{dt} + \lambda c = \frac{m\delta(t)}{V}$$

Particular solution:  $c = \frac{m}{v} e^{-\lambda t}$ 





#### Step loading (new continuos source)



Plot of (a) loading and (b) response for impulse loading

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## **UNSTEADY- SYSTEMS SOLUTION (CONT)**

#### Linear (Ramp) Loading

★ Linear function:  $W(t) = \pm \beta_l t$  (β<sub>l</sub>: rate of change[MT<sup>-2</sup>])

Particular solution : 
$$c = \pm \frac{\beta_1}{\lambda^2 v} \left( \lambda t - 1 + e^{-\lambda t} \right)$$



Plot of (a) loading and (b) response for a lineare increasing loading

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### Exponential loading

Exponential function:  $W(t) = W_e e^{\pm \beta_e t}$  ( $W_e$ : a parameter that denote the value at t = 0 [MT<sup>-1</sup>],  $\beta_e$ : growth rate (+) or decay (-) of loading [T<sup>-1</sup>])



Plot of (a) loading and (b) response for an exponential decaying loading





### Exercise 1:

<u>A</u> lake receives two sources of waste of a preserved pollutant from two plants with the following characteristics:

Source of waste from factory 1 with the load of pollutants with the following characteristics:

$$W(t) = \begin{cases} 0 & , x < 1930 \\ 13.2 \times 10^9 (t - 1930) & , 1930 \le t \le 1960 \end{cases}$$

Waste source from factory 2 with pollutant load has the following characteristics:

$$W(t) = \begin{cases} 0 & , x < 1900\\ 229 \times 10^9 e^{0.015(t-1900)} & , 1900 \le t \le 1960 \end{cases}$$

where W(t) has units g/year

The initial concentration of the lake is 3mg/l. Characteristics of the lake: outflow 49.1x10<sup>9</sup> m<sup>3</sup>/year, V=4880x10<sup>9</sup> m<sup>3</sup>. Determine the concentration of pollutants in the lake from 1900 to 1960.





### Solution:

Because chloride is a conservative substance.:

$$\lambda = \frac{Q}{V} = \frac{49.1 \times 10^9}{4880 \times 10^9} = 0.01 \ (yr^{-1})$$

From 1900 to 1930

$$c = 3 + \frac{229 \times 10^9}{4880 \times 10^9 (0.01 + 0.015)} \left( e^{0.015(t - 1900)} - e^{-0.01(t - 1900)} \right)$$

From 1930 to 1960





Concentration movement over time





### Exercise 2.

The lake has the following characteristics: Inflow = outflow =  $5 \times 10^5$  m<sup>3</sup>/year, volume =  $4 \times 10^7$  m<sup>3</sup>, surface area =  $5 \times 10^6$  m<sup>2</sup>. The initial concentration of the lake in a stable state is  $5 \mu g/l$ .

The lake receives two sources of waste as follows.:

- In 1994 the lake received a load of 500 kg/year from a fertilizer factory.
- In 1997, the lake began receiving waste from residential areas at a rate of population growth each year.  $p = 200e^{0.2t}$  and each citizen will generate phosphorus amounts of 0.5 kg per year.

Calculate the concentration of the lake from 1994 to 2010. Know the deposition speed of phosphorus is 8m /year.



## **LECTURE**

# **MODELLING THE MARINE ENVIRONMENT**







### Lecture 7

## **PROCESS OF SUBSTANCE TRANSMISSION**





### Lecture 7B

# **SYSTEM OF REACTOR**

Lecturer: Professor. TS. Nguyen Ky Phung Ms. Dang Thi Thanh Le





## Moving Impact System

- Mass Balance
- Solution for the stable state
- Solution for the unstable state

# Reponses Impact System

- Mass Balance
- Solution for the stable state
- Solution for the unstable state



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(a) Moving Impact System



(b) Reponses Impact System





# **Moving Impact System**



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A simple application is to simulate a chain of interconnected lakes using short river sections. In this case, we consider a simple system of two lakes as described:



Mass balance for these reactors can be written:

Lake 1 
$$V_1 \frac{dC_1}{dt} = W_1 + Q_{01}C_0 - Q_{12}C_1 - k_1V_1C_1$$
 (1)

Lake 2

 $V_2 \frac{dC_2}{dt} = W_2 + Q_{12}C_1 - Q_{23}C_2 - k_2V_2C_2$ (2)





At steady – state: 
$$a_{11}C_1 = W_1$$
 (3)  
-  $a_{21}C_1 + a_{22}C_2 = W_2$  (4)

where

$$a_{11} = Q_{12} + k_1 V_1$$
  $a_{21} = Q_{12}$   $a_{22} = Q_{23} + k_2 V_2$ 

Solution

Lake 1 
$$C_1 = \frac{1}{a_{11}} W_1 = \frac{1}{Q_{12} + k_1 V_1} W_1$$
 (5)

Lake 2 
$$C_2 = \frac{W_2 + a_{21}C_1}{a_{22}} = \frac{1}{Q_{23} + k_2V_2}W_2 + \frac{Q_{12}}{Q_{23} + k_2V_2}\frac{1}{Q_{12} + k_1V_1}W_1$$
 (6)





Example 1. Suppose that three lakes are connected in series. The pollutant settles at a rate of 10 m/yr.

(a) Determining concentrations in the steady- state of each reactor

(b) Determining how much the concentration in the third reactor to the loading of the second reactor.







(a) The concentration of the lakes is determined as follows:

$$C_{1} = \frac{W_{1}}{Q_{12} + vA_{1}} = \frac{2 \times 10^{9}}{1.0 \times 10^{6} + (10 \times 0.667 \times 10^{6})} = 260.76 \,\mu g L^{-1}$$

$$C_{2} = \frac{W_{2}}{Q_{12} + vA_{1}} + \frac{Q_{12}C_{1}}{Q_{12} + vA_{1}} = \frac{4 \times 10^{9}}{1.0 \times 10^{6} + (10 \times 0.571 \times 10^{6})} + \frac{1.0 \times 10^{6} (270.76)}{1.0 \times 10^{6} + (10 \times 0.571 \times 10^{6})} + \frac{1.0 \times 10^{6} (270.76)}{1.0 \times 10^{6} + (10 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} + \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} + \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} + \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} + \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} + \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 0.571 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 0.571 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})} = \frac{100 \times 10^{6} + (100 \times 10^{6})}{1.0 \times 10^{6} + (100 \times 10^{6})}$$

 $Q_{23} + vA_2 \quad Q_{23} + vA_2 \quad 1.0 \times 10^6 + (10 \times 0.571 \times 10^6)^+ 1.0 \times 10^6 + (10 \times 0.571 \times 10^6)^+$ = 596.13 + 38.86 = 634.99  $\mu gL^{-1}$ 

$$C_{3} = \frac{W_{3}}{Q_{34} + vA_{3}} + \frac{Q_{23}C_{2}}{Q_{34} + vA_{3}} = \frac{1 \times 10^{9}}{1.0 \times 10^{6} + (10 \times 1 \times 10^{6})} + \frac{1.0 \times 10^{6} (634.99)}{1.0 \times 10^{6} + (10 \times 1 \times 10^{6})}$$
$$= 148.64 \,\mu g L^{-1}$$

(b) As the solution to C2 above we notice.,  $596.13\mu gL^{-1}$  of C<sub>2</sub> due to load into lake 2 (W<sub>2</sub>), whereas  $38.86\mu gL^{-1}$  it is due to loading into lake 1. Therefore, the effect of Lake 2 on Lake 3 can be calculated as follows:

$$\frac{1.0 \times 10^{6} (596.13)}{1.0 \times 10^{6} + (10 \times 1 \times 10^{6})} = 54.19 \,\mu g L^{-1}$$





## **SOLUTION FOR THE STABLE STATE**

A special case for the system of well-mixed lakes is when the volume and flow of the lakes are the same



The solution of the lakes is simplified as follows

Lake 1 
$$C_1 = \frac{Q}{Q+kV}C_0$$

Lake 2 
$$C_2 = \frac{Q}{Q+kV}C_1 = \frac{Q}{Q+kV}\frac{Q}{Q+kV}C_0$$

Lake n 
$$C_n = \left(\frac{Q}{Q+kV}\right)^n C_0$$



Equations (1) and (2) in case W = 0 are written as follows:

Lake 1 
$$\frac{dC_1}{dt} = -\lambda_{11}C_1$$
 (7)  
Lake 2  $\frac{dC_2}{dt} = \lambda_{21}C_1 - \lambda_{22}C_2$  (8)  
Where  $\lambda_{11} = \frac{Q_{12}}{V_1} + k_1$   $\lambda_{21} = \frac{Q_{12}}{V_1}$   $\lambda_{22} = \frac{Q_{23}}{V_2} + k_2$ 

At t = 0:  $C_1 = C_{10}$  and  $C_2 = C_{20}$ , We have the following solution.:

Lake 1 
$$C_1 = C_{10} e^{-\lambda_{11}t}$$
 (9)

Lake 2 
$$C_2 = C_{20}e^{-\lambda_{22}t} + \frac{\lambda_{21}C_{10}}{\lambda_{22} - \lambda_{11}} \left( e^{-\lambda_{11}t} - e^{-\lambda_{22}t} \right)$$
 (10)

# SOLUTION FOR THE UNSTABLE STATE

To find a general solution to the system of lakes, Di Toro (1972) developed the following relationship:

Lake 1 
$$C_1(t, \lambda_{11}) = C_{10}e^{-\lambda_{11}t}$$

Lake2 
$$C_2(t, \lambda_{11}, \lambda_{22}) = \frac{\lambda_{21}}{\lambda_{22} - \lambda_{11}} [C_1(t, \lambda_{11}) - C_1(t, \lambda_{22})]$$

Lake 3 
$$C_3(t, \lambda_{11}, \lambda_{22}, \lambda_{33}) = \frac{\lambda_{32}}{\lambda_{33} - \lambda_{22}} [C_2(t, \lambda_{11}, \lambda_{22}) - C_1(t, \lambda_{11}, \lambda_{33})]$$

Lake 4 
$$C_4(t, \lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{44}) = \frac{\lambda_{43}}{\lambda_{44} - \lambda_{33}} [C_3(t, \lambda_{11}, \lambda_{22}, \lambda_{33}) - C_1(t, \lambda_{11}, \lambda_{22}, \lambda_{44})]$$

Lake n 
$$C_n(t, \lambda_{11}, ..., \lambda_{n,n}) = \frac{\lambda_{n,n-1}}{\lambda_{n,n} - \lambda_{n-1,n-1}} \left[ C_{n-1}(t, \lambda_{11}, ..., \lambda_{n-2,n-2}, \lambda_{n-1,n-1}) - C_{n-1}(t, \lambda_{11}, ..., \lambda_{n-2,n-2}, \lambda_{n,n}) \right]$$

The general form of this factored version is

$$C_{n}(t,\lambda_{11},...,\lambda_{n-1,n-1},\lambda_{n,n}) = \prod_{j=1}^{n-1} \lambda_{j+1,j} \sum_{i=1}^{n} \frac{C_{1}(t,\lambda_{i,i})}{\prod_{j=1(j\neq i)}^{n} (\lambda_{j,j} - \lambda_{i,i})}$$

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# **Reponses Impact System**





In this case, we consider a simple system of two lakes as described:



Mass balances for two CSTRs with feedback can be written

Lake 1 
$$V_1 \frac{dC_1}{dt} = W_1 + Q_{01}C_0 - Q_{12}C_1 - k_1V_1C_1 + Q_{21}C_2$$
 (11)  
Lake 2  $V_2 \frac{dC_2}{dt} = W_2 + Q_{12}C_1 - Q_{21}C_2 - Q_{23}C_2 - k_2V_2C_2$  (12)



(16)

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Solution Lake 1  $C_1 = \frac{1}{a_{11} - (a_{21}a_{12}/a_{22})}W_1 + \frac{1}{a_{21} - (a_{11}a_{22}/a_{12})}W_2$ (15)Lake 2  $C_2 = \frac{1}{a_{12} - (a_{13}a_{22}/a_{23})}W_1 + \frac{1}{a_{22} - (a_{23}a_{23}/a_{23})}W_2$ 

 $a_{11} = Q_{12} + k_1 V_1$  $a_{21} = -Q_{12}$  $a_{22} = Q_{21} + Q_{23} + k_2 V_2$  $a_{12} = -Q_{21}$ 

Where

At steady - state:

$$a_{11}C_1 + a_{12}C_2 = W_1 \tag{13}$$

$$a_{21}C_1 + a_{22}C_2 = W_2 \tag{14}$$





## The solution method for the system of reactor

Considering the response impact system of 3 lakes, the equation of the mass balance of system of reactor is written as follows:

$$a_{11}C_1 + a_{12}C_2 + a_{13}C_3 = W_1$$
(17)  
$$a_{21}C_1 + a_{22}C_2 + a_{23}C_3 = W_2$$
(18)  
$$a_{31}C_1 + a_{32}C_2 + a_{33}C_3 = W_3$$
(19)

The equation system is rewritten as follows:  $[A]{C} = {W}$  (20) where

$$\begin{bmatrix} A \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \qquad \{C\} = \begin{cases} C_1 \\ C_2 \\ C_3 \end{cases} \qquad \{W\} = \begin{cases} W_1 \\ W_2 \\ W_3 \end{cases}$$





## The solution method for the system of reactor (cont)

The solution of this equation system is as follows:  $\{C\} = [A]^{-1} \{W\}$  (21)

where [A]<sup>-1</sup> is an inverse matrix. [A]

Using the two-matrix method, the equation (20) can be deployed as follows:

$$C_{1} = a_{11}^{(-1)}W_{1} + a_{12}^{(-1)}W_{2} + a_{13}^{(-1)}W_{3}$$
(22)  

$$C_{2} = a_{21}^{(-1)}W_{1} + a_{22}^{(-1)}W_{2} + a_{23}^{(-1)}W_{3}$$
(23)  

$$C_{3} = a_{31}^{(-1)}W_{1} + a_{32}^{(-1)}W_{2} + a_{33}^{(-1)}W_{3}$$
(24)

Where  $a_{i,i}^{(-1)}$  is coefficient in row i, column j in inverse matrix.

Suppose that three lakes are connected in series



(a) If Q =  $1 \times 10^6$  m<sup>3</sup>/yr,  $\alpha$  = 0.5 and the rate of settles of pollutants is 10 m/yr. Calculate the concentration of each lake..

(b) Use an inverse matrix to determine the concentration of Lake 3 due to the load to Lake 2 contributing.

(c) Identify inverse matrix in case where  $\alpha = 0$ 





(a) The steady-state mass balances for the three reactors can be written as:

$$0 = W_{1} - (Q + \alpha Q)C_{1} - vA_{1}C_{1} + \alpha QC_{3}$$
  

$$0 = W_{2} + (Q + \alpha Q)C_{1} - (Q + \alpha Q)C_{2} - vA_{2}C_{2}$$
  

$$0 = W_{3} + (Q + \alpha Q)C_{2} - (Q + \alpha Q)C_{3} - vA_{3}C_{3}$$

Substituting the parameter values, the three simultaneous equations can be

expressed in matrix form as  $\begin{bmatrix} 8.17 \times 10^6 & 0 & -0.5 \times 10^6 \\ -1.5 \times 10^6 & 7.21 \times 10^6 & 0 \\ 0 & -1.5 \times 10^6 & 11.5 \times 10^6 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{bmatrix} 2 \times 10^9 \\ 4 \times 10^9 \\ 1 \times 10^9 \end{bmatrix}$ 

The inverse matrix is defined as follows

$$1.23 \times 10^{-7}$$
 $1.11 \times 10^{-9}$  $5.33 \times 10^{-9}$  $2.55 \times 10^{-8}$  $1.39 \times 10^{-7}$  $1.11 \times 10^{-9}$  $3.33 \times 10^{-9}$  $1.81 \times 10^{-8}$  $8.71 \times 10^{-8}$ 

Which can be multiplied by (W) to give

$$\begin{cases} C_1 \\ C_2 \\ C_3 \end{cases} = \begin{cases} 255 \\ 608 \\ 166 \end{cases}$$
 20





(b) The effect of lake 2 on the concentration of lake 3 is determined based on the coefficient  $a_{32}^{(-1)}$ .

$$a_{32}^{(-1)} = 1.81 \times 10^{-8} \,\mu g.L^{-1} \,/\,mg.yr^{-1}$$

The concentration of lake 3 due to the loading of lake 2 contributes: (1.81×10<sup>-8</sup>) × (4×10<sup>9</sup>) = 72.5  $\mu$ g/L

(c) Where  $\alpha = 0$ , The equation system is written as a matrix as follows:

$$\begin{bmatrix} 7.67 \times 10^6 & 0 & 0 \\ -1 \times 10^6 & 6.71 \times 10^6 & 0 \\ 0 & -1 \times 10^6 & 11 \times 10^6 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{bmatrix} 2 \times 10^9 \\ 4 \times 10^9 \\ 1 \times 10^9 \end{bmatrix}$$

The inverse matrix is defined as follows:

$$\begin{bmatrix} 1.30 \times 10^{-7} & 0 & 0 \\ 1.94 \times 10^{-8} & 1.49 \times 10^{-7} & 0 \\ 1.77 \times 10^{-9} & 1.35 \times 10^{-8} & 9.09 \times 10^{-8} \end{bmatrix}$$





Equations (11) and (12) in case W = 0 are written as follows:

Lake 1 
$$\frac{dC_1}{dt} = -\alpha_{11}C_1 + \alpha_{12}C_2$$
 (25)  
Lake 2  $\frac{dC_2}{dt} = \alpha_{21}C_1 - \alpha_{22}C_2$  (26)

Where

$$\alpha_{11} = \frac{Q_{12}}{V_1} + k_1 \qquad \alpha_{12} = \frac{Q_{21}}{V_1} \qquad \alpha_{21} = \frac{Q_{12}}{V_2} \qquad \alpha_{22} = \frac{Q_{23} + Q_{21}}{V_2} + k_2$$

At t = 0:  $C_1 = C_{10}$  và  $C_2 = C_{20}$ , then the general solution can be developed:

Lake 1 
$$C_1 = C_{1f} e^{-\lambda_f t} + C_{1s} e^{-\lambda_s t}$$
 (27)

Lake 2  $C_2 = C_{2f} e^{-\lambda_f t} + C_{2s} e^{-\lambda_s t}$  (28)





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#### Where

 $\lambda$  are eigenvalue and is defined as follows.

$$\frac{\lambda_f}{\lambda_s} = \frac{(\alpha_{11} + \alpha_{22}) \pm \sqrt{(\alpha_{11} + \alpha_{22})^2 - 4(\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21})}}{2}$$

And the coefficients is

$$C_{1f} = \frac{(\lambda_f - \alpha_{22})C_{10} - \alpha_{12}C_{20}}{\lambda_f - \lambda_s} \qquad C_{1s} = \frac{\alpha_{12}C_{20} - (\lambda_s - \alpha_{22})C_{10}}{\lambda_f - \lambda_s}$$
$$C_{2f} = \frac{-\alpha_{21}C_{10} + (\lambda_f - \alpha_{11})C_{20}}{\lambda_f - \lambda_s} \qquad C_{2s} = \frac{-(\lambda_s - \alpha_{11})C_{20} + \alpha_{21}C_{10}}{\lambda_f - \lambda_s}$$

Based on the general solution, we realize that the resilience of the system depends on the magnitude of its own values. Note that  $\lambda_f > \lambda_s$  và  $\lambda_{f}$ ,  $\lambda_{s}$  Often used to refer to eigenvalues "fast" and "slow".





**Example, 3.** For a system of 2 lakes with the same characteristics as shown as below.



(a) If  $Q = 1 \times 10^6$  m<sup>3</sup>/yr,  $\alpha = 0.5$  and the rate of settles of pollutant is10 m/yr. Determined the concentration of each lake.

(b) Use the concentration value calculated in sentence (a) as the original value, determining the concentration movement over time of each lake.





(a) The solution is similar to example 2, the concentration in the steady- state of each lake:  $\{C\} = \begin{cases} 1224.5 \\ 898 \end{cases}$ 

(b) The concentration of each lake over time is determined as follows

$$C_1 = 981.24e^{-10.04t} + 243.25e^{-0.61t}$$
$$C_2 = -15.67e^{-10.04t} + 913.63e^{-0.61t}$$

The chart shows the concentration of each lake as follows



Based on the graph, because of the large eigenvalue of Lake 1 at the beginning, the Lake 1 concentration rapidly decreased before slowly recovered



## **LECTURE**

# **MODELLING THE MARINE ENVIRONMENT**







### Lecture 7

## THE SUBSTANCE TRANSMISSION PROCESS





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### **Lecture 7C**

# CALCULATION METHODOLOGY PROFICIENT FUSION SYSTEMS





- Euler Method
- Heun Method
- Runge-Kutt Method

# Limitations of the analytical method



- Non Idealized loading functions: Usually using the ideal load functions to achieve a closed solution. Although pollutant loads rarely acquire those functions, most are in any form and unpattern
- Variable parameter: In the previous chapters, there is a hypothesis that model parameters such as Q, V, k, etc. are constant. The reality shows that these parameters often change over time.
- Multiple–Lake systems: The system that consists of more than 2 lakes uses computers to accomplish an effective solution.
- Non-linear kinetics: Despite the vital of first-order kinetics, some water quality problems will require these kinetic reactions to be in a nonlinear state, or the analytical solutions are not acquired.





The complete mixed lake model

$$\frac{dC}{dt} = \frac{W(t)}{V} - \lambda C \tag{1}$$

where

$$\lambda = \frac{Q}{V} + k + \frac{v}{H} \tag{2}$$

Use the forward difference, we can approximate the first derivative of c with respect to t by :

$$\frac{dC_i}{dt} \cong \frac{\Delta C}{\Delta t} = \frac{C_{i+1} - C_i}{t_{i+1} - t_i}$$
(3)

Substituting (3) into the equation (1):

$$\frac{C_{i+1} - C_i}{t_{i+1} - t_i} = \frac{W(t)}{V} - \lambda C_i$$
(4)





$$C_{i+1} = C_i + \left[\frac{W(t)}{V} - \lambda C_i\right] (t_{i+1} - t_i)$$
(5)

This method can be generalized as follows:

 $C_{i+1} = C_i + f(t_i, C_i)h$ (6)С Where  $f(t_i, C_i) = dC_i/dt$  Tthe dư báo sai số value calculated at t<sub>i</sub> và C<sub>i</sub>, đúng  $vah = t_{i+1} - t_{i}$  $C_i$  $\frac{dc_i}{dt}$ h ti  $t_{i\pm 1}$ t 7




**Example 1.** A well-mixed lake has the following characteristics:  $Q = 10^5$  m<sup>3</sup>/yr,  $V = 10^6$  m<sup>3</sup>, z = 5 m,  $k = 0.2yr^{-1}$ , v = 0.25 m/yr.

At t = 0, the lake receives a loading of  $50 \times 10^6$  g/yr and the lake has an initial concentration is 15 mg/L. Use the Euler method to simulate the concentration from the moment t = 0 to 20 year. With a time step of 1 year, Compare the results with the analytical solution:

$$C = C_0 e^{-\lambda t} + \frac{W}{\lambda V} \left( 1 - e^{-\lambda t} \right)$$





(a) Eigenvalue is calculated as follows

$$\lambda = \frac{10^5}{10^6} + 0.2 + \frac{0.25}{5} (yr^{-1})$$

At the beginning (t =0), the concentration of the lake is 15 mg/L and receive a loading is  $50 \times 10^6$  g/yr.

At t=1 year

$$C(1) = 15 + \left[\frac{50 \times 10^6}{10^6} - 0.35(15)\right] \times 1.0 = 59.75(mg/l)$$

At t=2 year  $C(2) = 59.75 + \left[\frac{50 \times 10^{6}}{10^{6}} - 0.35(59.75)\right] \times 1.0 = 88.8375(mg/l)$ 



Graph comparing the euler method solution and the analytical solution

t (yr)	C (mg/L)		t (yr)	C (mg/L)	
	PP Euler	Analytical		PP Euler	Analytical
		method			method
0	15.00	15.00	6	133.22	127.20
1	59.75	52.75	7	136.59	131.82
2	88.84	79.37	8	138.78	135.08
3	107.75	98.12	9	140.21	137.38
4	120.04	111.33	10	141.14	139.00
5	128.03	120.64	$\infty$	142.86	142.86

HEUN METHOD



One method to improve the error in the Euler method is to identify the derivative on either side of a time step - one at the beginning  $(t_i)$  and one at the end  $(t_{i+1})$ . These two derivative components are then taken on average to estimate the slope of the entire time step (h)



Graphical describing the Heun method





The Heun method is also known as the forecasting-calibratation method. This method is summarized as follows:

Forecast:

$$C_{i+1}^{0} = C_{i} + f(t_{i}, C_{i})h$$
(7)

Calibratation *h*:

$$C_{i+1} = C_i + \frac{f(t_i, C_i) + f(t_{i+1}, C_{i+1}^0)}{2}h$$
(8)

**Example 2.** A well-mixed lake has the following characteristics:  $\mathbb{Q}^{\text{Co-funded by the property of the p$ 

At t = 0, the lake receives a loading of  $50 \times 10^6$  g/yr and the lake has an initial concentration is 15 mg/L. Use the Huen method to simulate the concentration from the moment t = 0 to 20 year With a time step of 1 year. Compare the results with the analytical solution :

$$C = C_0 e^{-\lambda t} + \frac{W}{\lambda V} \left( 1 - e^{-\lambda t} \right)$$





(a) Eigenvalue is calculated as follows

$$\lambda = \frac{10^5}{10^6} + 0.2 + \frac{0.25}{5} (yr^{-1})$$

At the beginning (t =0) The concentration of the lake is 15 mg/L and receive a loading  $50x10^6$  g/yr.

At t=1 year

$$C^{0}(1) = 15 + (50 - 0.35 \times 15) \times 1 = 59.75(mg/l)$$
$$C(1) = 15 + \frac{(50 - 0.35 \times 15) + (50 - 0.35 \times 59.75)}{2} \times 1 = 51.92(mg/l)$$

The same solution for other times



Graph comparing the solution by the Heun method and the Analytical

	solution							
t (yr)	C (mg/L)		t (yr)	C (mg/L)				
	PP Heun	Analytical		PP Heun	Analytical			
		method			method			
0	15.00	15.00	6	126.31	127.20			
1	51.92	52.75	7	131.09	131.82			
2	78.18	79.37	8	134.49	135.08			
3	96.86	98.12	9	136.91	137.38			
4	110.14	111.33	10	138.63	139.00			
5	119.59	120.64	$\infty$	142.86	142.86			





 $t_{i+1}$ 

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 $C_{i+1} = C_i + \phi h$ (9)The Runge-Kutta method is generalized.:

 $\phi$  is the slope (commonly referred to as the home function)

The most commonly used Runga-Kutta method is the 4th order method and has the following form: . . . .





Butcher et al. (1964) developed the 5step Runge-Kutta method as follows:

$$C_{i+1} = C_i + \left[\frac{1}{90}\left(7k_1 + 32k_3 + 12k_4 + 32k_5 + 7k_6\right)\right]h$$
(11)

where

$$\begin{aligned} k_{1} &= f\left(t_{i}, C_{i}\right) \\ k_{2} &= f\left(t_{i} + \frac{1}{4}h, C_{i} + \frac{1}{4}hk_{1}\right) \\ k_{3} &= f\left(t_{i} + \frac{1}{4}h, C_{i} + \frac{1}{4}hk_{1} + \frac{1}{8}hk_{2}\right) \\ k_{4} &= f\left(t_{i} + \frac{1}{2}h, C_{i} - \frac{1}{2}hk_{2} + hk_{3}\right) \\ k_{5} &= f\left(t_{i} + \frac{3}{4}h, C_{i} + \frac{3}{16}hk_{1} + \frac{9}{16}hk_{4}\right) \\ k_{6} &= f\left(t_{i} + h, C_{i} - \frac{3}{7}hk_{1} + \frac{2}{7}hk_{2} + \frac{12}{7}hk_{3} - \frac{12}{7}hk_{4} + \frac{8}{7}hk_{5}\right) \end{aligned}$$





**Example 3.** A well-mixed lake has the following characteristics:  $Q = 10^5$  m<sup>3</sup>/yr,  $V = 10^6$  m<sup>3</sup>, z = 5 m,  $k = 0.2yr^{-1}$ , v = 0.25 m/yr.

At t = 0, the lake receives a loading of  $50x10^6$  g/yr and the lake has an initial concentration is 15 mg/L. Use the Runnge method to simulate the concentration from the moment t = 0 to 20 year With a time step of 1 year. Compare the results with the Analytical method :

$$C = C_0 e^{-\lambda t} + \frac{W}{\lambda V} \left( 1 - e^{-\lambda t} \right)$$





The above methods described can easily be adapted to simulate a system of difference equations of the form of:

$$\frac{dC_1}{dt} = f_1(C_1, C_2, ..., C_n)$$
(12)  
$$\frac{dC_2}{dt} = f_2(C_1, C_2, ..., C_n)$$
(13)  
$$\frac{dC_n}{dt} = f_n(C_1, C_2, ..., C_n)$$
(14)

To solve this equation system, there is requires "n" as the initial condition at the time of starting the calculation





**Exercise 1.** A 5kg spill of dissolved pesticides occurred in Lake 1 in a system of two lakes. Know that both lakes are perfectly mixed. The characteristics of the lake are as follows:

	Lake 1	Lake 2
Volume (m <sup>3</sup> )	0.5×10 <sup>6</sup>	0.6×10 <sup>6</sup>
Output (m <sup>3</sup> /yr)	1×10 <sup>6</sup>	1×10 <sup>6</sup>

The concentration over time of the two lakes is forecast using the Euler method. Compare the results with the analytical solution and present the results by the graph.



## **LECTURE**

# **MODELLING THE MARINE ENVIRONMENT**

Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le







## Lecture 7

## **PROCESS OF SUBSTANCE TRANSMISSION**

Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le





# Lecture 7D ADVECTION AND DISUSION





## **ADVECTION AND DISUSION**

- Advection: Advection results from flow that is unidirectional and does not change the iden tity of the substance being transported. As in Figure advection moves matter from one position in space to another
- Diffusion: Refer to the moment of the mass due to random water motion or mixing
  - Molecular diffusion
  - Turbulent diffusion









#### ✤ Experiment







Mass equation balance for lake1:

$$V_1 \frac{dC_1}{dt} = D'(C_2 - C_1)$$

Where:

 $V_1$ 

D'





- : Lake volume 1;
- $C_1, C_2$  : concentration of 1 and 2;
  - : Diffusion [m<sup>3</sup>/năm]





## Three factors affect diffusion:

- The mixing flow D' reflects the intensity of the mixing. Thus, if the tanks was subjects to only weak mixing such as due to Brownian motion, D' would be small. If it were subjected to vigorous phýical mixing, D' would be large
- Mass transport is directly proportional to the interface area
- Mass transport is proportional to the difference in concentration between the two lakes (gradient concentration)
- Diffuse to the right if  $C_1 > C_2$ 
  - + Diffuse to the left if C1 < C2
  - + Do not diffuse if C1 = C





**Example 1.** Simulation of the time required for the experiment described on Figure 2 to be completed 95%. Lời giải:

Mass balance equation

$$\frac{V}{2} \frac{dC_1}{dt} = D'(C_2 - C_1)$$
  
V<sub>1</sub> = V<sub>2</sub>, :  $C_{10} = C_1 + C_2$ 

Mass balancing equations at the moment:







physicist Adolf 1855, In introduced the diffusion model:

$$J_x = -D\frac{dC}{dx}$$

Fick

Where:

flux in the mass Х x ditection[ML<sup>-2</sup>T<sup>-1</sup>]

D: diffusion coefficient [L<sup>2</sup>T<sup>-1</sup>]

Fick's Law: Mass flux is proportional to the gradient (that is, the derivative or rsate of change)



Graphical depictions the effect of concentration gradients on the mass flux. 8





## Determination of diffusion coefficient



In diffusion, two important quantities are d diffusion coefficient and blend length I. For the molecular, the parameter is defined [LT<sup>-1</sup>]:

$$v_d = \frac{D}{l}$$
 where  $v_d$  is called a diffusion mass – transfer coefficient

For, **Turbulent diffusion** :  $E' = \frac{EA_c}{1}$ 







Mass balancing equation:

Μ 12

Main  
lake 
$$V_1 \frac{dC_1}{dt} = W_1 - Q_1 C_1 - k_1 V_1 C_1 + Q_2 C_2 + E'(C_2 - C_1)$$
  
Bay  $V_2 \frac{dC_2}{dt} = W_2 - Q_2 C_2 - k_2 V_2 C_2 + E'(C_1 - C_2)$ 

 $\sim$ 





## Estimation of Diffusion

Conservatve are substances that do not have a decomposition process. (k=0)

Mass balance for the bay(2):

$$V_2 \frac{dC_2}{dt} = W_2 - Q_2 C_2 + E' (C_1 - C_2)$$

Steady – state slotions

$$E' = \frac{W_2 - Q_2 C_2}{C_2 - C_1}$$





#### Example 2: For a lake and bay, parameters presented in the table

	BAY		LAKE		
Volume	V <sub>2</sub>	8	V <sub>1</sub>	3507	10 <sup>9</sup> m <sup>3</sup>
Depth	$H_2$	5.81	H <sub>1</sub>	60.3	m
Surface area	$A_2$	1,376	A <sub>1</sub>	58,194	10 <sup>6</sup> m <sup>2</sup>
Outflow	$Q_2$	7	Q <sub>1</sub>	161	10 <sup>9</sup> m <sup>3</sup> yr <sup>-1</sup>
Chloride	$C_2$	15.2	<b>C</b> <sub>1</sub>	5.4	g m <sup>-3</sup>
concentration					
Chloride loading	$W_2$	0.353	W <sub>1</sub>	0	10 <sup>12</sup> g yr <sup>-1</sup>
Phosphours	$W_{p2}$	1.42	W <sub>p1</sub>	4.05	10 <sup>12</sup> mg yr <sup>-1</sup>
loading	F		F -		

Note that the mass diffusion coefficient is determined based on the concentration gradient of Chlo (preservative). Determine the diffusion coefficient and mass-transfer coefficient for the process.





$$E' = \frac{0.353 \times 10^{12} - [7 \times 10^9 \times 15.2]}{15.2 - 5.4} = 25.2 \times 10^9 \ m^3 / n \breve{a} m$$

Mass- transfer coefficient:

$$v_d = \frac{E'}{A_c} = \frac{25.2 \times 10^9}{0.17 \times 10^6} = 1.48 \times 10^5 \, m/n$$
ăm

**Diffusion coefficient** 

$$E = v_d l = 1.48 \times 10^5 \times 10 \times 10^3 = 1.48 \times 10^9 m^2 / n \breve{a} m$$





#### Example 3: For a lake and bay, parameters presented in the table

	BAY		LAKE		
Volume	V <sub>2</sub>	8	V	3507	- 10 <sup>9</sup> m <sup>3</sup>
Depth	$H_2$	5.81	H <sub>1</sub>	60.3	m
Surface area	$A_2$	1,376	A <sub>1</sub>	58,194	10 <sup>6</sup> m <sup>2</sup>
Outflow	$Q_2$	7	Q <sub>1</sub>	161	10 <sup>9</sup> m <sup>3</sup> yr <sup>-1</sup>
Chloride	$C_2$	15.2	C <sub>1</sub>	5.4	g m <sup>-3</sup>
concentration					
Chloride loading	$W_2$	0.353	W <sub>1</sub>	0	10 <sup>12</sup> g yr <sup>-1</sup>
Phosphours	$W_{p2}$	1.42	W <sub>p1</sub>	4.05	10 <sup>12</sup> mg yr <sup>-1</sup>
loading	•		r		

For the deposition rate of phosphorus is v = 16 m/yr. Determine (a) the concentration of inflows, (b) the concentration in the stable state of the lake and bay.



Solution



4.05 x 1012

 $Q_{1,in} = Q_1 - Q_2 = 161 \times 10^9 - 7 \times 10^9 = 154 \times 10^9 \, m^3 \, yr^{-1}$ 

Inflow concentration



$$C_2 = \frac{1}{2.373 \times 10^{12}} W_{p1} + \frac{1}{5.345 \times 10^{12}} W_{p2} = 1.705 + 26.658 = 28.36 \mu g L^{-1}$$



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## Diffusion

Mass is spreads via random molecular motion or due to large-scale agitation in the water environment.

- There are two important differences.:
- + Turbulent motion is greater than the random molecular motion, therefore mixing caused by tangle diffusion is greater than molecular diffusion.
- + Molecular diffusion takes place uniformly at scale, while Turbulent diffusion takes place in wider-sized ranges. Therefore, diffusion depends on space.





## Dispersion

Dispersion involves the process of causing pollutants to spread out. This process is the result of a change in the flow velocity through space.





# **ADDITIONAL TRANSPORT MECHANISMS (cont)**

## CONDUCTION AND CONVECTION

Conduction and convection are two pro- cesses that originate from heat transfer and aerodynamics that are roughly analogous to diffusion and advection

- Conduction refers to the transfer of heat by molecular activity from one sub-stance to another or through a substance
- **Convection** which generally refers to the motions in a fluid that result in the transport and mixing of the fluid's properties, takes two forms.
  - Free convection refers to vertical atmospheric motions due to the buoyancy of heated or cooled fluid, For example in meteorology, the rising of heated surface air and sinking of cooler air aloft is called "free convection
  - Forced convection is due to external forces. An example is the • lateral movement of heat or mass due to the wind. Thus forced convection is akin to advection



## **LECTURE**

# **MODELLING THE MARINE ENVIRONMENT**

Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le







## Lecture 8

## **BOD AND OXYGEN SATURATION**

Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le





- The cycle organic decomposition and production
- Saturated dissolved oxygen
- Experiment
- Biochemical Oxygen Demand (BOD)
- BOD model for tributaries
- DO saturation

RGANIC MATTER DECOMPOSITION AND PRODUCTION CY Continued by the Ensemble Programme



The cycle above can be described by chemical equations:

$$6CO_2 + 6H_2O \xrightarrow{\text{photosynthesis}}_{\text{respiration}} C_6H_{12}O_6 + 6O_2$$





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The organic matter decomposition cycle is described by the following chemical equation:

$$C_6H_{12}O_6 + 6O_2 \xrightarrow{\text{Respiratory}} 6CO_2 + 6H_2O_2$$

Mass balancing equation:

Glucose:  $V \frac{dg}{dt} = -k_1 Vg$ 

Oxy: 
$$V\frac{do}{dt} = -r_{og}k_1Vg$$

k<sub>1</sub>: rate of decomposition [1/day]

r<sub>og</sub>: the stoichiometric of oxygen consumed to glucose decomposition (mg O/mg-glucose)





**Example 1:** Put 2mg of glucose in a 250ml bottle, then add a small amount of bacteria. Fill the bottle with water and close the lid. The initial oxygen level was 10mgL<sup>-1</sup>. If glucose breaks down at a rate of 0.1/day, determine the concentration of oxygen as a function over time in this experiment.





#### Solution:

Initial concentration of glucose

$$g_0 = \frac{2 \text{ mg}}{250 \text{ mL}} \left(\frac{1000 \text{ mL}}{\text{L}}\right) = 8 \text{mg/L}$$

stoichiometry:

$$r_{og} = \frac{6(32)}{6 \times 12 + 1 \times 12 + 6 \times 16} = 1.0667 \text{ mgO/mg glucose}$$

Glucose levels break down and oxygen depletion over time:

$$g = 8e^{-0.1t}$$
  
o = 10 - 8.5333(1 - e^{-0.1t})



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- Siochemical oxygen demand (BOD) is the amount of oxygen needed for microorganisms to oxidize organic matter over a certain period of time.
- Mass balancing equation for oxidizing organic matter in the bottle:

✤ V  $\frac{dL}{dt} = -k_1 VL$ L: the amount of oxidized organic matter left in the bottle: [mgO L<sup>-1</sup>]

At t = 0:  $L = L_0$  Experiment with the equation now.

$$L = L_0 e^{-k_1 t}$$

Amount of oxygen consumed during decomposition:

$$y = L_0 - L \rightarrow y = L_0 (1 - e^{-k_1 t})$$

Where y is BOD (mgO  $L^{-1}$ );  $L_0$  is the initial concentration of oxidized organic matter (expressed in units of oxygen) or ultimate BOD

#### BIOCHEMICAL OXYGEN DEMAND (BOD BUSH Programme European Union

Mass balance equation for oxygen:

$$V\frac{do}{dt} = -k_1 V L_0 e^{-k_1 t}$$

At t = 0:  $o = o_0$ , the solution of the equation





The L0 value is the initial concentration of dissolved organic matter or final BOD





# Mass balance equation for a Stream $\frac{dL}{dt} = -U\frac{dL}{dx} - k_r L \label{eq:mass_state}$

 $k_r$  = total removal rate (d^-1) includes the process of decomposition and sttling,  $k_r = k_d + k_s$ 

In a steady - state

$$0 = -U\frac{dL}{dx} - k_r L$$

Let's say at the point of discharge, the mixing process is complete.

$$L_0 = \frac{Q_w L_w + Q_r L_r}{Q_w + Q_r}$$

Tại t = 0:  $L = L_0$  the solution as below

$$\mathbf{L} = \mathbf{L}_0 \mathbf{e}^{-\frac{k_r}{U}x}$$





#### **Exercises**

A discharge stream (flow 2 cms, BOD is 10 mg/l) from an active sludge treatment plant poured into a river (flow 5 cms and BOD is 0 mg/l). Characteristics of the river:  $k_{r.} 20 = 0.2$  days-1, cross-section area is 25 m<sup>2</sup>, and T = 28°C,  $\theta$  =1,047 for BOD decomposition.

a. Determination of BOD levels at the mixing point

b. How far is the distance from the discharge point so that the BOD concentration reaches 5% of the original BOD valu?



#### The effect of temperature. (APHA 1992)

$$\ln o_{sf} = -139.34411 + \frac{1.575701.10^5}{T_a} - \frac{6.642308.10^7}{T_a^2} + \frac{1.243800.10^{10}}{T_a^3} - \frac{8.621949.10^{11}}{T_a^4}$$

 $o_{sf}$  Is the concentration of do saturation at the pressure 1 atm (mg L<sup>-1</sup>) and T<sub>a</sub> is absolute temperature. (K), T<sub>a</sub> = T + 273.15

#### Effects of salinity (APHA 1992)

$$\ln o_{ss} = \ln o_{sf} - S \left( 1.7674.10^{-2} - \frac{1.0754.10^{1}}{T_{a}} + \frac{2.1407.10^{3}}{T_{a}^{2}} \right)$$
  
o\_{ss} is the concentration of do saturation in seawater at pressure 1 atm (mgL<sup>-1</sup>), S is salinity (gL<sup>-1</sup> or ppt).

S=1.80655 x Chlor

Chlor is a concentration of chloride (ppt). The higher the salinity, the lower the amount of oxygen in the water.





### Effects of pressure (APHA 1992)

$$o_{sp} = o_{si} p \left[ \frac{\left(1 - \frac{p_{wv}}{p}\right) \left(1 - \theta p\right)}{\left(1 - p_{wv}\right) \left(1 - \theta\right)} \right]$$

p = atmospheric pressure (atm);

o<sub>sp</sub> = saturated oxygen concentration at pressure p (mg L<sup>-1</sup>);

 $o_{s1}$  = saturation concentration of dissolved oxygen at pressure 1 atm (mgL<sup>-1</sup>);  $p_{wv}$  = partial pressure part of steam (atm)

$$\ln p_{wv} = 11.8571 - \frac{3840.70}{T_a} - \frac{216.961}{T_a^2} \qquad \theta = 0.000975 - 1.426.10^{-5}T + 6.436.10^{-8}T^2$$

Zison el at (1978) advanced approximation formula based on altitude  $o_{sp} = o_{s1} [1 - 0.1148 * elev(km)]$ 





#### **Exercises**

DO, temperature, and salinity are measured at an estuaries as follows:

Distance from the sea	30	20	10
Temperature, °C	25	22	18
Salinity, ppt	5	10	20
DO	5	6.5	7.5

Calculate the percentage of saturated oxygen at the above 3 locations



### **LECTURE**

# **MODELLING THE MARINE ENVIRONMENT**

Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le







#### Lecture 9

# **STRETER- PHELPS MODEL**

Lecturer: Prof. Nguyen Ky Phung MSc. Dang Thi Thanh Le





# Point source

Distribution source





# STRETER- PHELPS POINT SOURCES





Mass balance equation:

BOD:  $V \frac{dL}{dt} = -k_d VL$ 

DO:  $V \frac{do}{dt} = -k_d VL + k_a V(o_s - o)$ 

- DO Deficit:  $D = o_s o \longrightarrow \frac{dD}{dt} = -\frac{do}{dt}$
- $\rightarrow V \frac{dD}{dt} = k_d VL k_a VD$ If at = 0: L = L<sub>o</sub> and D = O, above equation can be differentiated L = L<sub>0</sub>e<sup>-k\_dt</sup>

$$D = \frac{k_{d}L_{0}}{k_{a} - k_{d}} \left( e^{-k_{d}t} - e^{-k_{a}t} \right)$$







BOD decomposition process in (a) closed and (b) open system

**POINTS SOURCE -STREETER-PHELPS EQUATION** 

A stream with a single-point source of BOD. The river segment is in a steady state and is characterized by plug flow with constant hydrological and geometry (PFR system). This is the simplest manifestation of the classic Streeter – Pheld model

Mass balance: 
$$0 = -U \frac{dL}{dx} - k_r L$$

$$0 = -U \frac{dD}{dx} + k_d L - k_a D$$
với k<sub>r</sub> = k<sub>d</sub> + k<sub>s</sub> 0 x

If L = L<sub>o</sub> và D = D<sub>o</sub> at t = 0, then these equation can be solved for  $L = L_0 e^{-\frac{k_r}{U}x}$   $D = D_0 e^{-\frac{k_a}{U}x} + \frac{k_d L_0}{k_o - k_r} \left( e^{-\frac{k_r}{U}x} - e^{-\frac{k_a}{U}x} \right)$ 

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#### Some formulas calculate reaeration coefficient (k<sub>a</sub>)

O'Connor-Dobbins (1956)

$$k_a = 3.93 \frac{U^{0.5}}{H^{1.5}}$$

Churchill (1962)

$$k_a = 5.026 \frac{U}{H^{1.67}}$$

Owens và Gibbs (1964)

$$k_a = 5.32 \frac{U^{0.67}}{H^{1.85}}$$

where:  $k_a$  (1/day), U (m/s), H (m)



#### Example 1:

0 km



The river is described as shown in the picture. The de-oxygenation rate for CBOD is 0.5 day<sup>-1</sup> in 20°C. From a distance of 20 km downstream from the plant, the CBOD deposition rate is 0.25 day<sup>-1</sup>.

 $Q_t = 1.157 \text{ m}^3/\text{s}$  Assuming that O'Connor-Dobbins's  $T_t = 15^\circ \text{ C}$  reaeration formula is used, calculates the concentration of DO in the system.

#### MARE The hydrographic morphological parameters and reaction kinetics of the system



Parameter	Units	KP > 100	KP: 100-60	KP < 60
Depth	m	1.19	1.24	1.41
Area	m²	14.71	15.5	18.05
Flow	m <sup>3</sup> s <sup>-1</sup>	5.787	6.250	7.407
	m <sup>3</sup> d <sup>-1</sup>	500,000	540,000	640,000
Velocity	m s⁻¹	0.393	0.403	0.410
	m d <sup>-1</sup>	33,955	34,891	35,524
Parameter	KP > 100	KP: 100 - 80	KP: 80 - 60	KP < 60
T (°C)	20	20.59	20.59	19.72
T (°C) O <sub>s</sub> (mgL <sup>-1</sup> )	20 9.092	20.59 8.987	20.59 8.987	19.72 9.143
T (°C) $O_{s}$ (mgL <sup>-1</sup> ) $k_{a}$ (d <sup>-1</sup> )	20 9.092 1.902	20.59 8.987 1.842	20.59 8.987 1.842	19.72 9.143 1.494
T (°C) $O_{s}$ (mgL <sup>-1</sup> ) $k_{a}$ (d <sup>-1</sup> ) $k_{r}$ (d <sup>-1</sup> )	20 9.092 1.902 0.50	20.59 8.987 1.842 0.764	20.59 8.987 1.842 0.514	19.72 9.143 1.494 0.494





With a diffusion system such as an estuary the Streeter-Phelps equation can be written as:

$$0 = E \frac{d^2 L}{dx^2} - U \frac{dL}{dx} - k_r L$$
$$0 = E \frac{d^2 D}{dx^2} - U \frac{dD}{dx} + k_d L - k_a D$$

If  $L = L_o var D = D_o at t = 0$ , the solution for BOD is

$$\begin{split} L &= L_0 e^{j_{1r}x} & x \leq 0 \\ L &= L_0 e^{j_{2r}x} & x \geq 0 \end{split}$$



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The solution to oxygen deficiency

$$D = \frac{k_d}{k_a - k_r} \frac{W}{Q} \left( \frac{e^{j_1 r x}}{\alpha_r} - \frac{e^{j_1 a x}}{\alpha_a} \right) \qquad x \le 0$$
$$D = \frac{k_d}{k_a - k_r} \frac{W}{Q} \left( \frac{e^{j_2 r x}}{\alpha_r} - \frac{e^{j_2 a x}}{\alpha_a} \right) \qquad x \ge 0$$

where

$$L_{0} = \frac{W}{\alpha_{r}Q}$$

$$\alpha_{r} = \sqrt{1 + \frac{4k_{r}E}{U^{2}}}$$

$$\alpha_{a} = \sqrt{1 + \frac{4k_{a}E}{U^{2}}}$$

$$\frac{j_{1r}}{j_{2r}} = \frac{U}{2E} \left( 1 \pm \alpha_r \right)$$

٠

$$\frac{J_{1a}}{J_{2a}} = \frac{U}{2E} \left( 1 \pm \alpha_a \right)$$





DO chart for a point waste source into an estuary

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**Exercises 1:** Determine BOD and DO for the following section of the river.

For the decomposition rate of BOD at 20°C is 0.35 (1/day),  $\theta$  = 1.047.







# STRETER- PHELPS DISSTRIBUTED SOURCES

PARAMETERIZATION OF DISTRIBUTION SOUR CES of the European Union

Mass balance in case of plug- flow:

$$0 = -U\frac{dc}{dx} - kc + S_d$$

If at = 0:  $c = c_o$ , then the solution is:

$$c = \frac{S_d}{k} \left( 1 - e^{-kt} \right)$$

 $S_d$  = the rate of the distribution source. (ML<sup>-3</sup>T<sup>-1</sup>).

t = travel time , t = x/U.



PARAMETERIZATION OF DISTRIBUTION SOURCES

#### Distributed source types



- L = distribution source length
- V = volume
- $A_c$  = the cross-section area of the segment in which the source is included.





 Source: bottom sludge with high organic concentration Mass balance:

$$0 = -U\frac{dL}{dx} - k_{\rm r}L + S_{\rm L}$$

Where  $S_L$  = the speed of the BOD distribution source(gm<sup>-3</sup>d<sup>-1</sup>)

 $k_r$  = rate of BOD removal (day<sup>-1</sup>).

Solution when t = 0: L = 0:

$$L = \frac{S_L}{k_r} \left( 1 - e^{-k_r t} \right)$$





The mass balance for oxygen deficiency is written as follows

$$0 = -U\frac{dD}{dx} - k_a D + \frac{k_d}{k_r} S_L \left(1 - e^{-k_r t}\right)$$

At t = 0: D = 0, The solution to mass balance is as follows:

$$D = \frac{k_{d}S_{L}}{k_{r}k_{a}} \left(1 - e^{-k_{a}t}\right) - \frac{k_{d}S_{L}}{k_{r}(k_{a} - k_{r})} \left(e^{-k_{r}t} - e^{-k_{a}t}\right)$$

Where t = travel time. (t = x/U)





- Source: Plants (photosynthesis)
- Deposition: plants (respiration), SOD
- Mass balance

$$0 = -U\frac{dD}{dx} - k_a D - P + R + \frac{S_B}{H}$$

Where P, R: the rate of photosynthesis and respiration of plants (gm<sup>-3</sup>nday<sup>-1</sup>)

 $S_{R}$  = oxygen demand rate for sediment (gm<sup>-2</sup>day<sup>-1</sup>)

H = depth(m)

• The solution when t = 0: L = 0:

$$D = \frac{-P + R + (S_{B}'/H)}{k_{a}} (1 - e^{-k_{a}t})$$



General solution to the points and distribution sources of BDO and



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#### **Exercises:**

**D**etermine bod and do for the following section of the river.

<u>_</u>					
$L_0 = 80 \text{ mg/L}$ <b>SOD = 2 gm</b>		²day⁻¹	P - R =	P - R = 1 gm <sup>-2</sup> day <sup>-1</sup>	
		gm <sup>-2</sup> day <sup>1</sup>			
	0	20 km	40 km	60 km	<b></b>
U (mps) H (m)	0.1 0.8	0.15 1		0.1 1	
k <sub>r</sub> (ngày <sup>-1</sup> )	0.2	0.1		0.1	
κ <sub>d</sub> (ngày ') k <sub>a</sub> (ngày⁻¹)	1	1.2		1.2	
o <sub>s</sub> (mgL <sup>-1</sup> )	10	9		8	