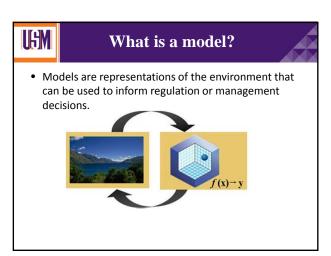
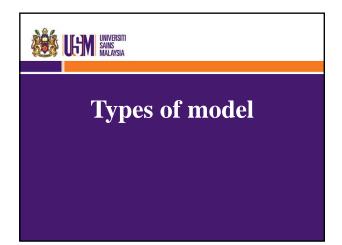


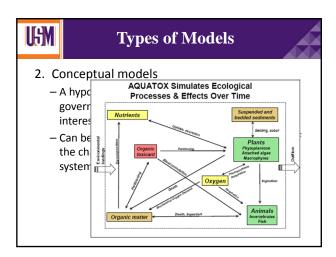
What is a model?

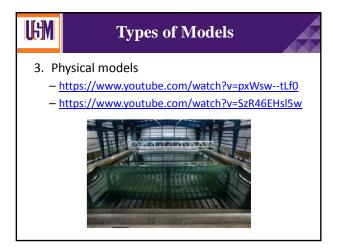
- A model is defined as (EPA, 2009):
- " A simplification of reality that is constructed to gain insights into select attributes of a physical, biological, economic, or social system. A formal representation of the behavior of system processes, often in mathematical or statistical terms. The basis can also be physical or conceptual."

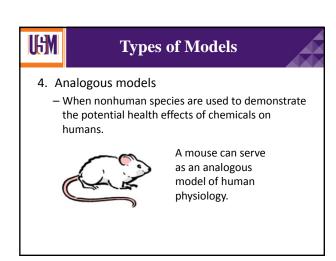


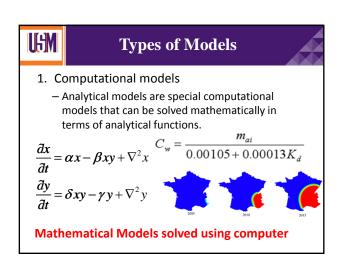


Types of Models 1. Computational models 2. Conceptual models 3. Physical models 4. Analogous Models

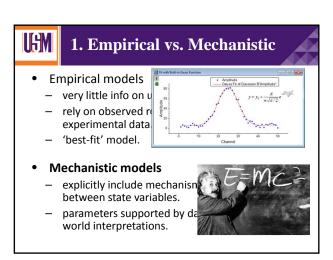








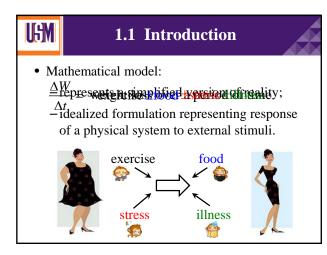
Computational Models 1. Empirical vs. Mechanistic models 2. Deterministic vs. Probabilistic models 3. Dynamic vs. Static models

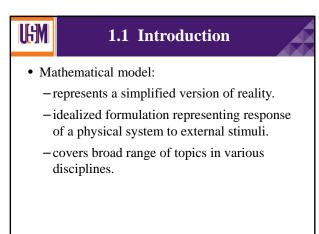


Deterministic vs. Probabilistic Deterministic models

- provide solution of state variable
- do not explicitly simulate data 'uncertainty'.
- repeated simulation ⇒ consistent results.
- Probabilistic models
 - Statistical/stochastic models.
 - evaluate impact of variability and uncertainty in various input parameters.

Dynamic vs. Static Dynamic models Changes with time or space. For most situations, where a differential equation is being approximated, the simulation model will use a finite time step (or spatial step) to estimate changes in state variables over time (or space). Static models make predictions about the way a system changes as the varue or an independent variable changes.





1.1 Introduction

- Environmental Modeling.
- The term environment covers a myriad of possible systems and processes, including land, ocean and atmospheric based systems.
- Specifically water quality modeling.

Water Quality (WQ) Model

- Built generally for the following reasons:
 - To gain a better understanding of the fate and transport of chemicals by quantifying their reactions, speciation and movement.
 - 2. To determine chemical exposure concentrations to aquatic organisms and/or humans in the past, present or future.
 - 3. To predict future conditions under various loading scenarios or management action alternatives.

Water Quality (WQ) Model

- 1. To gain a better understanding of the fate and transport of chemicals by quantifying their reactions, speciation and movement.
- Could provide answer to the questions:
 - -Where do all the pollutants go?
 - Are they with us forever?
- -How rapidly are they degraded?
- Related to the fate, transport and persistence of pollutants in the environment.

UEM

Water Quality (WQ) Model

- 2. To determine chemical exposure concentrations to aquatic organisms and/or humans in the past, present or future.
- Safe level of frequency and duration of exposure to the chemical pollutants;



Pertains to assessing environmental risk and impact.

USM

Water Quality (WQ) Model

- To predict future conditions under various loading scenarios or management action alternatives.
- Assess potential concentrations;
- Under various loading scenarios;



- Regardless of availability of monitoring data;
- Always desirable to have estimate of concentrations under various conditions.



Water Quality (WQ) Model

• Important:

No existing mathematical models provide a <u>perfectly</u> accurate and complete picture of reality.

- Tradeoffs: accuracy, flexibility and cost;
- Offer important insights and info;
- About the nature and scope of a problem;
- And can inform solutions.



Water Quality (WQ) Model

Four ingredients are necessary:

- Field data on chemical concentrations and mass discharge inputs;
- 2. A mathematical formulation;
- Rate constants and equilibrium coefficients for the mathematical model;
- 4. Some performance criteria with which to judge the model,



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1.2 Model Calibration and Verification

- Field data are needed for model calibration and verification;
- Depending on the ultimate use of the model;
- Amount of field reconnaissance varies;
- Model for regulatory purposes;
- Should have enough field data to be confident of the model results.

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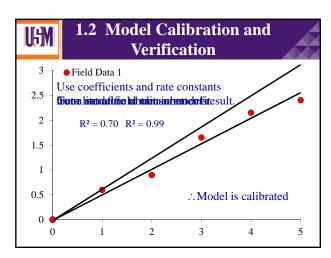
1.2 Model Calibration and Verification

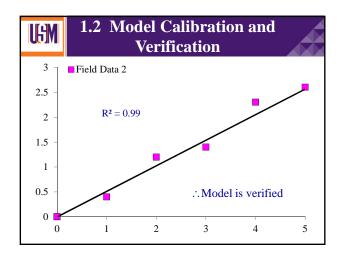
- This requires two sets of field measurements;
 - One for model calibration;
 - One for verification under different circumstances;
- Comparison between simulation results and field measurements;
- Coefficients and rate constants from literature or laboratory studies;
- Flow discharge rates as input to drive model;

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1.2 Model Calibration and Verification

- Statistical comparison between the model results and field measurements;
- If errors are not acceptable, tune the model to obtain an acceptable simulation;
- Model tuning = systematically varies rate constants and coefficients;
- Within the range of experimentally determined values reported in the literature.
- Thus the model is calibrated.





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Definitions for Model Calibration and Verification

- Mathematical model a quantitative formulation of chemical, physical and biological processes that simulates the system.

 Mathematical model a quantitative $\frac{dC}{dT} = kC$
- **State variable** the dependent variable that is being modeled (in this context, usually a chemical concentration).
- **Model parameters** coefficients in the model that are used to formulate the mass balance equation (e.g. rate constants, equilibrium constants)

UGM

Definitions for Model Calibration and Verification

- **Model inputs** forcing functions or constants required to run the model (e.g. flow rate, input chemical concentrations).
- Calibration a statistically acceptable comparison between model results and field measurements; adjustment or "tuning" of model parameters is allowed within the range of experimentally determined values reported in the literature.

Definitions for Model Calibration and Verification

- **Verification** a statistically acceptable comparison between model results and a second (independent) set of field data for another year or at an alternate site; model parameters are fixed and no further adjustment is allowed after the calibration step.
- **Simulation** use of model with any input data set (even hypothetical input) and not requiring calibration or verification with field data.

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Definitions for Model Calibration and Verification

- Validation scientific acceptance that (1) the model includes all major and salient processes, (2) the processes are formulated correctly and (3) the model suitably describes observed phenomena for the use intended.
- **Robustness** utility of the model established after repeated applications under different circumstances and at different sites.

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Definitions for Model Calibration and Verification

- **Post audit** a comparison of model predictions to future field measurements at that time.
- **Sensitivity analysis** determination of the effect of a small change in model parameters on the results (state variable), either by numerical simulation or mathematical techniques.



Definitions for Model Calibration and Verification

• Uncertainty analysis – determination of the uncertainty (standard deviation) of the state variable expected value (mean) due to uncertainty in model parameters, inputs, or initial state via stochastic modeling techniques.



1.2 Model Calibration and Verification

- How "good" the model results are depends on desired use of the model or predictions;
- Criteria for acceptance of calibration or verification depend on intended use of model;
- Acceptance of a model calibration or verification does not necessarily imply that the model, itself, is validated.



1.2 Model Calibration and Verification

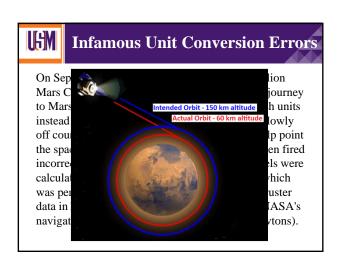
- It is possible that the model works well under one set of circumstances but poorly under another;
- As the model is applied to different situations at various locations, we gain confidence in the model and its robustness;
- Repeated model testing is crucial to gaining confidence in the model and to understanding its limitations.

1.3 Basic Measurement and Unit

- Understanding basic measurement and unit;
- An important aspect of math. modeling;
- A unit is necessary to communicate values of that physical quantity;
- Communicating a measurement without a unit is impossible because a measurement cannot be described without a reference used to make sense of the value given.

Table 1.1 Basic measurement and unit in SI (M = mass, L = length, T = time)					
Measure ment	e Dimen sion	Unit	Measure ment	Dimen sion	Unit
Length	L	m	Time	T	S
Area	L^2	m^2	Conc.	M L-3	kg/m ³ , kgm ⁻³
Volume	L^3	m^3	Loading	M T-1	kg/s
Mass	M	kg	Kinetic rate	T-1	s ⁻¹

Table 1.2 Some common unit conversions Measurement Conversion $1 \text{ km} = 10^3 \text{ m}$ Length $1 \text{ m} = 10^2 \text{ cm}$ 1 cm = 10 mm1 m = 3.28 ftVolume $1 \text{ m}^3 = 1000 \text{ L}$ 1 L = 1000 mL1 kg = 1000 gMass 1 g = 1000 mg1 kg = 2.2 lbs



M£U

Infamous Unit Conversion Errors

On January 26, 2004 at Tokyo Disneyland's Space Mountain, an axle broke on a roller coaster train midride, causing it to derail. The cause was a part being the wrong size due to a conversion of the master plans in 1995 from English units to Metric units. In 2002, new axles were mistakenly ordered using the pre-1995 English specifications instead of the current Metric specifications.

English Unit
Mile
Kilometer
Foot Meter
Inch Centimeter
Pound Grams
Ounce Grams
Gallon Liter
Cestims Kelvin



UEM

Infamous Unit Conversion Errors

On 23 July 1983, Air Canada Flight 143 ran completely out of fuel about halfway through its flight from Montreal to Edmonton. Fuel loading was miscalculated through misunderstanding of the recently adopted metric system. For the trip, the pilot calculated a fuel requirement of 22,300 kilograms, and they wanted to know how much in liters should be pumped. They used 1.77 as their density ratio in performing their calculations. However, 1.77 was given in pounds per liter, not kilograms per liter. The correct number should have been 0.80 kilograms/liter;

thus, their final figure accounted for less than half of the necessary fuel.



1.3 Basic Measurement and Unit

- Units can only be added or subtracted if they are the same type;
- But it can always be multiplied or divided;
- A physical value can be expressed in various units;
- E.g., measurement of length can be expressed in meter (m) or centimeter (cm), among others.
- Conversion of units is required to compare physical quantities in different units.

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Example 1.1(a)

• What do we have if we add 1 km to 3 kg?

We cannot add items of different measurements.



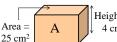




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Example 1.1(b)

• Box A has an area of 25 cm² and a height of 4 cm. Box B has a volume of 80. Which one of these boxes has a larger volume?



Height = 4 cm



Volume $= 80 \text{ cm}^3$

Box A volume = $25 \times 4 = 100 \text{ cm}^3$.

Folko Brivoils moet is is 80 ncamed them Boxe Achan at Langerave Inetween Box B volume and Box A volume.

UEM

Example 1.1(c)

• Between 2.2 pounds of iron rods and 1 kg of cotton buds, which one of these is heavier?

> Both are of the same weight. 2.2 pounds = 1 kg







USM

Example 1.1(d)

• Lina has a 300 g packet of jelly beans and 0.25 kg of lollipops for her kid's birthday party. What is the total weight of the sweet treats that she has for the party?





Lollipops = $0.25 \text{ kg} = 0.25 \times 1000 \text{ g} = 250 \text{ g}$ Total weight = 550 g or 0.55 kg.

USM

Example 1.1(e)

• Convert kg/m³ to mg/L.

$$1 \text{ kg} = 10^6 \text{ mg}$$

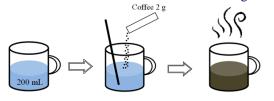
$$1 \text{ m}^3 = 10^3 \text{ L}$$

$$\therefore 1 \text{ kg/m}^3 = 10^6/10^3 \text{ mg/L}$$

= 1000 mg/L

Example 1.2

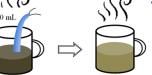
- Consider a cup with 200 mL of water.
- Two grams of coffee powder from a sachet is added to the cup of water.
- After stirring the beverage, find the concentration of coffee in kg/m³ in that cup of water.



USW

Example 1.2

- The color of the beverage indicates that the coffee may be too strong.
- Therefore, another 50 mL of water is added into the beverage.
- After stirring the beverage, find the diluted concentration of coffee in kg/m³ in that cup of 8 kg/m^3





1.4 Conservation of Mass and the Mass Balance

- To model aquatic channel systems;
- We begin with a simple mass balance based upon the principle of continuity:

Matter is neither created nor destroyed in macroscopic chemical, physical and biological interactions.









USM

1.4 Conservation of Mass and the Mass Balance

- In quantitative terms, the principle is expressed as a mass-balance equation;
- Accounts for all transfers of matter across the Transport Insystem boundaries and all transformation out occurring within the system;
 - For a finite period of time,

Accumulation = loadings ± transport ± reactions

• For situations where more than two substances interact, additional equations could be written.



1.4 Conservation of Mass and the Mass Balance

Accumulation = loadings ± transport ± reactions

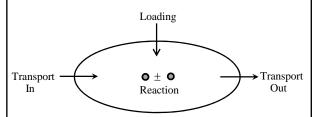


Figure 1.1 Schematic representation of the loading, transport and reaction of a substance moving though and reacting within a volume of water.

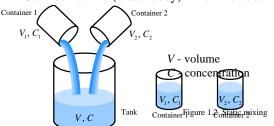
UGM

1.4 Conservation of Mass and the Mass Balance

- System can then be divided into subvolumes;
- Levels of substances at various locations within the volume;
- Math. division of space and matter into compartments = segmentation;
- Fundamental to the application of mass conservation to water quality problems;
- Concept of segmentation will be discussed further in Chapter 3.

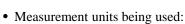
1.4 Conservation of Mass and the Mass Balance

- Conservation of mass and the mass balance in simpler systems;
- Control volume (water body) in form of a tank.



1.4 Conservation of Mass and the Mass Balance

• Volume V and concentration C after mixing of the two liquids in the tank can be determined;

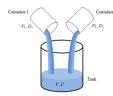


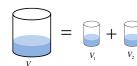
- meter (m) for length, kilogram (kg) for mass and second (s) for time;
- Area = m^2 , volume = m^3 ;
- concentration = kg/m³;

1.4 Conservation of Mass and the Mass Balance

• The law of conservation of volume states that the total volume *V* after mixing is

$$V = V_1 + V_2$$
, m³ (1.1)





(1.3)

UEM

1.4 Conservation of Mass and the Mass Balance

- Masses M_1 and M_2 for both liquids are $M_1 = C_1V_1$ and $M_2 = C_2V_2$ kg
- Concentrations C_1 and C_2 in kg/m³ (or kgm⁻³);
- Law of conservation of mass states that the total mass *M* of the mixture is conserved as

$$M = M_1 + M_2$$
, kg (1.2)

or
$$CV = C_1 V_1 + C_2 V_2$$
, kg (1.3)

USM

1.4 Conservation of Mass and the Mass Balance

• Here, *C* is the concentration of the liquid in the tank after complete mixing.

$$V = V_1 + V_2$$
 (1.1)

$$C \hat{V} = C_1 V_1 + C_2 V_2$$

$$\Rightarrow C(V_1 + V_2) = C_1 V_1 + C_2 V$$

$$\therefore C = \frac{C_1 V_1 + C_2 V_2}{V_1 + V_2} , \text{ kg/m}^3 \quad (1.4)$$



1.4 Conservation of Mass and the Mass Balance

• In short, the liquid concentration *C* after complete mixing is given by

$$C = \frac{M}{V} = \frac{\text{mass}}{\text{volume}} \left(\frac{\text{kg}}{\text{m}^3}\right)$$
 (1.5)

UGM

1.4 Conservation of Mass and the Mass Balance

- $V = V_1 + V_2$, m³ states that volume is conserved;
- $M = M_1 + M_2$, kg states that mass is conserved;
- Complete mixing process is in static state;
- Indicating that steady state has been achieved;
- After complete mixing, the state of the liquid *no longer depends on time*;
- i.e. volume *V*, mass *M* and concentration *C* do not change from time to time.

USM

1.4 Conservation of Mass and the Mass Balance

- On contrary, if the state of the liquid *changes* with time, then we called this a *dynamic state*;
- Dynamic mixing process will be discussed next with time dependency emphasized by the notation (t), e.g. V(t) and C(t).

USM

1.4 Conservation of Mass and the Mass Balance

- Suppose at time t sec, liquid in a tank has a volume of V m³ and concentration C kg/m³;
- Liquid flows into this tank at the flow rate of Q_1 m³/s and with a concentration of C_1 kg/m³;
- Liquid also $c_i(t)$ flows out of this tank at the flow rate of Q_2 m³/s and concentration of C_2 kg/m³.

Figure 1.3 Dynamic mixing



UGM

1.4 Conservation of Mass and the Mass Balance

- Laws of conservation of mass and volume are used to obtain the formulations of volume *V* and concentration *C* of the liquid in the tank;
- Both variables *V* and *C* are time dependent, i.e.

$$V = V(t)$$
 $C = C(t)$

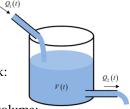
• To find V(t) and C(t), we observe what happen in a short time step Δt .

USM

1.4 Conservation of Mass and the Mass Balance

 ΔV = change in volume within Δt ΔM = change in mass within Δt • Volume flowing into tank:

 $Q_1 \Delta t$ m³



- Volume flowing out of tank: $Q_2\Delta t$ m³
- : law of conservation of volume:

$$\Delta V = Q_1 \ \Delta t - Q_2 \ \Delta t = (Q_1 - Q_2) \Delta t$$
 (1.6)
or
$$\frac{\Delta V}{\Delta t} = Q_1 - Q_2, \quad \text{m}^3/\text{s}$$



1.4 Conservation of Mass and the Mass Balance

$$\frac{\Delta V}{\Delta t} = Q_1 - Q_2 , \text{ m}^3/\text{s}$$

• Taking that $\Delta t \rightarrow 0$:

$$\frac{dV}{dt} = Q_1 - Q_2$$
, m³/s (1.7)

USW

1.4 Conservation of Mass and the Mass Balance

- Liquid flows into the tank:
 - flow rate of Q_1 m³/s.
 - concentration of C_1 kg/m³.
- \therefore mass input rate is $C_1 Q_1 \text{ kg/s}$;
- Unit for $C_1 Q_1$ is the product of $kg/m^3 \cdot m^3/s = kg/s$
- : change of mass in time step Δt is

$$(C_1 Q_1 \Delta t - C_2 Q_2 \Delta t)$$
 kg

USM

 $Q_{2}(t), C_{2}(t)$

V(t), C(t)

1.4 Conservation of Mass and the Mass Balance

- Initial mass in the tank is $M = C \cdot V$;
- ∴ change in mass is

$$\Delta M = \Delta (C \cdot V) = (C_1 Q_1 - C_2 Q_2) \Delta t \quad (1.8)$$

i.e.,
$$\frac{\Delta(C \cdot V)}{\Delta t} = C_1 Q_1 - C_2 Q_2$$

or
$$\frac{d}{dt}(C \cdot V) = C_1 Q_1 - C_2 Q_2$$
, kgs⁻¹ (1.9)

USM

1.4 Conservation of Mass and the Mass Balance

- Every term in Eqn (1.9) has the unit kgs⁻¹;
- Eqn (1.7) describes change in volume with time;
- Eqn (1.9) gives the change in mass (and subsequently change in concentration) with time.

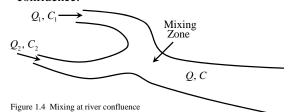
$$\frac{dV}{dt} = Q_1 - Q_2 , m^3/s$$
 (1.7)

$$\frac{d}{dt}(C \cdot V) = C_1 Q_1 - C_2 Q_2 , \text{ kgs}^{-1} (1.9)$$

USM

1.4 Conservation of Mass and the Mass Balance

Concept of ^C Eqn_V(1, V₂) on the resulted concentration from static mixture of liquids can be extended for the dynamic mixing at river confluence.



USM

1.4 Conservation of Mass and the Mass Balance

- Let:
 - $-Q_1$ = flow of a matter in river;
 - $-C_1$ = concentration of a matter in river;
 - $-Q_2$ = flow of a matter in river tributary;
 - $-C_2$ = conc. of a matter in river tributary;
- Complete mixing is achieved at mixing zone.

USM

1.4 Conservation of Mass and the Mass Balance

• By assuming that the mixing happens in **one second**, Equations (1.1) and (1.4) become

$$-V = V_1 + V_2 (1.1)$$

$$\longrightarrow Q = Q_1 + Q_2 , m^3 s^{-1} (1.10a)$$

$$C = \frac{C_1 V_1 + C_2 V_2}{V_1 + V_2}$$
 (1.4)

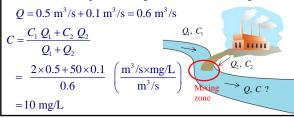
$$C = \frac{C_1 Q_1 + C_2 Q_2}{Q_1 + Q_2} , \text{ kg m}^{-3}$$
 (1.10b)

• With Q and C as the flow and concentration after complete mixing.

USW

Example 1.3

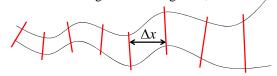
A river with the flow rate $Q_1 = 0.5 \text{ m}^3/\text{s}$ and chemical concentration $C_1 = 2 \text{ mg/L}$ receives an industrial effluent with the flow rate $Q_2 = 0.1$ m³/s and concentration $C_2 =$ 50 mg/L. Find the flow Q and the concentration C in the river after complete mixing is achieved at mixing zone.



USWI

1.5 Simple River Flow

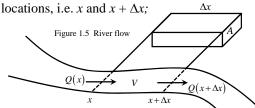
- Concept of the conservation of volume can be applied to river flow to formulate the flow in simpler form;
- Since the condition of a river can be different from one location to another, the river is divided into segments of length Δx ;



UGM

1.5 Simple River Flow

• To facilitate discussion, let us consider a segment of the river located between two



• For this small segment, let V = volume, W = width and D = depth.

1.5 Simple River Flow

- Let Q(x) m³/s = water flow at x;
- $Q(x + \Delta x)$ m³/s = water flow at $(x + \Delta x)$;
- In time step Δt :
- $Q(x) \cdot \Delta t = \text{amount of water that flows into the}$
- segment; $Q(x) \cdot \Delta t = \frac{m^3}{s} \times s = m^3$ $Q(x + \Delta x) \cdot \Delta t = \text{amount of water that flows out of the segment.}$ $Q(x + \Delta x) \cdot \Delta t = \frac{m^3}{s} \times s = m^3$

UGM

1.5 Simple River Flow

• .: conservation of volume dictates that

$$\Delta V = Q(x) \cdot \Delta t - Q(x + \Delta x) \cdot \Delta t$$

$$= \left[Q(x) - Q(x + \Delta x) \right] \cdot \Delta t$$

$$-\Delta Q$$

$$\Delta V = -\Delta Q \cdot \Delta t , m^{3}$$
 (1.11)

with $\Delta Q = Q(x + \Delta x) - Q(x)$.

USM

1.5 Simple River Flow

• Now, segment volume $V = \mathbf{A} \cdot \Delta x$



• Δx m = length of river segment;

 $A = W \cdot D$

• $\therefore \Delta V = \Delta (A \cdot \Delta x) = \Delta A \cdot \Delta x$

• $A \text{ m}^2 = \text{cross-sectional area};$

• \Rightarrow a change in volume ΔV will lead to a change in the cross sectional area ΔA .

$$\Delta A \cdot \Delta x = -\Delta Q \cdot \Delta t$$

UGM

1.5 Simple River Flow

$$\Delta A \cdot \Delta x = -\Delta Q \cdot \Delta t$$

$$\Rightarrow \frac{\Delta Q}{\Delta x} = -\frac{\Delta A}{\Delta t} \tag{1.12}$$

• By taking $\Delta x \to 0$ and $\Delta t \to 0$:

$$\frac{\partial Q}{\partial x} = -\frac{\partial A}{\partial t} \tag{1.13}$$

USM

1.5 Simple River Flow

$$\frac{\partial Q}{\partial x} = -\frac{\partial A}{\partial t} \tag{1.13}$$

- A partial differential equation (continuity equation) involving two variables Q(x, t) and A(x, t);
- To complete this system, another PDE (momentum equation) is needed.

USM

1.5 Simple River Flow

- The momentum equation is derived from the law of conservation of momentum;
- Newton's 2nd Law:
- Force = mass · acceleration $F = m \cdot a$ [kg m s⁻²] = [kg]·[m/s²]
- Further details available in Koh (2004);
- This system of PDE derived from the laws of conservation of mass and momentum is known as hydraulics model.

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1.5 Simple River Flow

- Hydrologic model refers to a system in which the momentum equation is replaced with a simpler approximation;
- Hydrologic models, in general, are easier to solve;
- When certain assumptions are applied, $\frac{\partial \mathcal{L}}{\partial x} = -\frac{\partial \mathcal{L}}{\partial t}$ Eqn (1.13) can be further simplified so that a complete and yet simple solution can be obtained (Koh, 2004).

