

is.

3.1 Segmentation and Model Resolution

- Aside from space and matter, there is a temporal aspect to segmentation;
- Related to the fact that mass balance defines changes in water body over a finite period of time;
- Model describes additional spatial and material detail by using more segments;
- † temporal focus: shorter "finite period" or *time step* for mass balance computation;
- *Model resolution:* degree to which space, time and matter are segmented.

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Model Resolution

- ≈ photography (Camera's lens focus);
- At times the foreground is important;
- At other times distant details might be of interest.







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Significance of Model Resolution for WQ analysis

- Two basic ways:
 - 1. Fine-scale phenomenon may have a direct, causative influence on predictions made on the coarser scale;



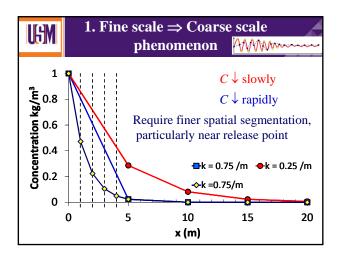
2. Influence of the problem context on the choice of scales.

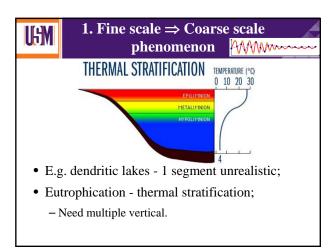


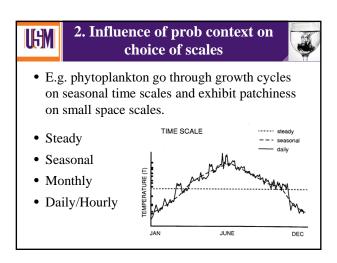
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1. Fine scale ⇒ Coarse scale phenomenon A

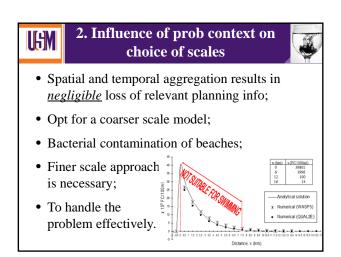
- Primarily a function of substance's properties and physical characteristics of the system;
- E.g. certain pollutants (e.g. enteric bacteria) die rapidly upon entering a water body;
- ∴ typically at ↑ levels near sewage discharge;
- \downarrow rapidly \Rightarrow background levels in open waters;
- Near-shore model of bacterial pollution;
- Require relatively fine spatial and temporal segmentation around sewage outfalls.







Put WQ planner might not have the funds to develop models to simulate such short-term variability; Often occur when large numbers of small lakes were being evaluated.



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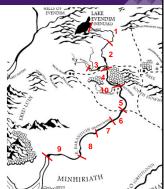
3.1 Segmentation and **Model Resolution**

- Temporal, spatial and kinetic scales of a problem often are interrelated;
- Fast kinetic processes, e.g. jet mixing of thermal effluents or bacterial die-off;
- Tend to manifest themselves on local (i.e. small) time and space scales;
- Problems with slow reactions, e.g. decay of persistent contaminants;
- Important on whole-system, long-term basis.

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3.2 Finite Segment Method

- Water body is often ÷ into a series of computational elements called segments;
- To account for variations over the water body;
- Levels of substances at various locations;



3.2 Finite Segment Method

- Best not to have too many segments than necessary;
- Imply a greater level of detail than is generally possible to parameterize;
- Greater opportunity for error (modify param);
- Comp. less efficient;
- · Calibration difficult.

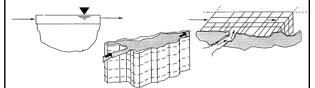
Segmentation Considerations

- Spatial scale of the problem
 - -Segment of a water body (e.g., reach, embayment)
 - -Whole water body (e.g., main river, lake, estuary)
 - -Whole river basin network



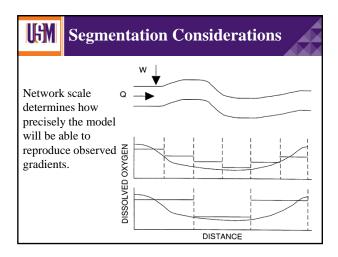
Segmentation Considerations

- Dimensionality and spatial discretization of segments
 - -Box, 1-, 2-, 3-dimensions
 - -Horizontal: tens of meters to tens of kilometers
 - Vertical: whole water column to tens of cm;



Segmentation Considerations

- Physical components
 - -Water column (epilimnion, hypolimnion)
 - -Benthic sediments (surface, subsurface)
- Model limitations
 - -Maximum # of Segments 3000
 - -Maximum # of Time Pairs 4000



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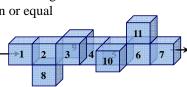
3.2 Finite Segment Method

- FSM segmentation of model ecosystems;
- Into various "completely mixed" boxes;
- Of known volume and interchange;
- Process known as compartmentalization;
- Popular assumption in fate modelling;
- Because assumption of complete mixing;
- Reduces the set of PDEs (in time and space);
- To one of ODEs (in time only).

3.2 Finite Segment Method

- Nevertheless, it is possible to recover some coarse spatial information;
- By introducing a number of interconnected segments/compartments;
- Interchange between segments is simulated via bulk dispersion or equal counterflows

between segments.

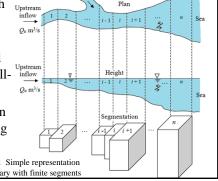


3.2 Finite Segment Method Estuary width Upstream inflow gradually 1 towards sea;

 Laterally and vertically wellmixed;

 Concentration gradient along the *x*-axis.

> Figure 3.1 Simple representation of an estuary with finite segments



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3.2 Finite Segment Method

- A substance reaction in a water body is important aspect of the substance's fate in the environment;
- But an equally important process has to do with the rate of a substance's transport in the aquatic environment;
- A substance is transported by water movement and may undergo additional transport processes such as decay or sedimentation.

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Transport Processes

• Decay – substance reduced in mass due to decomposition or sedimentation;

• Advection - sub movement at current velocity;



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Diffusion and Dispersion

 Diffusion: process where a constituent moves from a higher concentration to a lower concentration.







time

- Dispersion:
 - process by which substance is mixed within water column.
 - mixing caused by physical processes.

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Dispersion

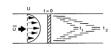
- 3 processes contribute to mixing (dispersion):
 - 1. Molecular diffusion, Random motion of particles



2. Turbulent diffusion, and Turbulent mixing of particles



Dispersion.
 Mixing caused
 by variations in velocities



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1. Molecular diffusion



- Mixing of dissolved substances;
- Due to random walk of molecules within fluid;
- Caused by kinetic energies of molecular vibrational, rotational and translational motion;
- In essence, molecular diffusion corresponds to an increase in entropy;
- Move from regions of high concentration to regions of low concentration;
- According to Fick's laws of diffusion.



1. Molecular diffusion



- Generally not an important process;
- In the transport of dissolved substances in natural waters;
- Except relating to transport through thin and stagnant films;
- At the air-water interface or transport through sediment pore water.



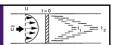
2. Turbulent diffusion



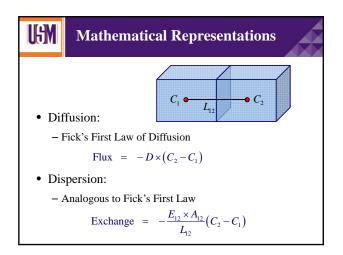
- @ Eddy diffusion;
- Mixing of dissolved substances caused by microscale turbulence;
- Advective process at microscale level caused by eddy fluctuations in turbulent shear flow;
- Shear forces within the body of water are sufficient to cause this form of mixing;
- Several orders of magnitude > mol. diffusion;
- A contributing factor in dispersion.



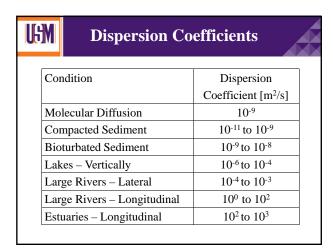
3. Dispersion

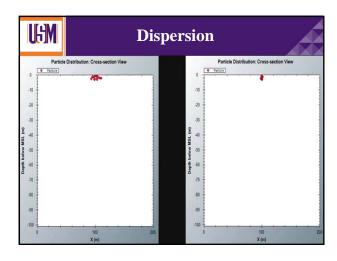


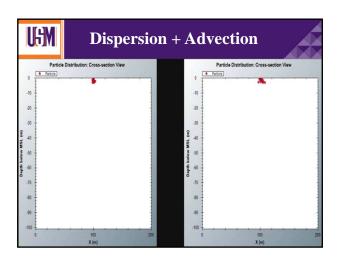
- Interaction of turbulent diffusion with velocity gradients;
- Caused by shear forces in the water body;
- Greater degree of mixing known as dispersion;
- Transport of substances in streams and rivers;
- Is predominantly by advection;
- But transport in lakes and estuaries is often dispersion-controlled.

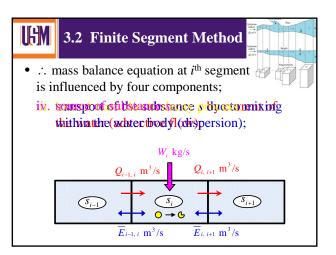


UGM	Range of Values for Dispersion		
Process		Direction	Typical Range [m ² /s]
Molecular Diffusion		Vertical	10 ⁻⁸ to 10 ⁻⁹
		Lateral	10 ⁻⁸ to 10 ⁻⁹
		Longitudinal	10 ⁻⁸ to 10 ⁻⁹
Turbulent Diffusion		Vertical	10 ⁻⁶ to 10 ⁻²
		Lateral	10 ⁻² to 10 ²
		Longitudinal	10 ⁻² to 10 ²
Dispersion		Vertical	10 ⁻³ to 10 ⁻¹
		Lateral	10 ⁻² to 10 ⁰
		Longitudinal	10 ⁻¹ to 10 ⁴



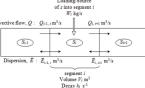






3.2 Finite Segment Method

- : mass balance equation at *i*th segment is influenced by four components;
 - i. transport of the substance s by current of the water (advective flow);
 - ii. transport of due to mixing within the water body (dispersion);
 - iii. loss of mass due Advective flow, Q: Q:1, i m3/5 to decay process;
 - iv. source of substance s.



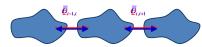
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3.2 Finite Segment Method

$$V_{i} \frac{dS_{i}}{dt} = Q_{i-1,i} S_{i-1,i} - Q_{i,i+1} S_{i,i+1} - k_{i} V_{i} S_{i} + W_{i}$$

$$+ \overline{E}_{i-1,i} \cdot (S_{i-1} - S_{i}) - (\gamma V + \nu A_{s}) C$$

$$+ \overline{E}_{i,i+1} \cdot (S_{i+1} - S_{i}) - kVC$$



Segment i-1

Segment i

Segment i+1

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(i) Advective Flow

- Mass per unit time for s that enters and exits segment i due to advective flow Q m³/s;
- Input of mass kg/s from upstream segment:

$$+Q_{i-1, i} \cdot s_{i-1, i} = +Q_{i-1, i} \cdot s_{i-1} \quad (3.1)$$

$$\left(\frac{\mathbf{m}^{3}}{\mathbf{s}}\right) \cdot \left(\frac{\mathbf{kg}}{\mathbf{m}^{3}}\right) = \left(\frac{\mathbf{kg}}{\mathbf{s}}\right)$$



USM

(i) Advective Flow

• Transport of mass by advective flow that exits segment i:

$$-Q_{i, i+1} \cdot s_{i, i+1} = -Q_{i, i+1} \cdot s_i$$
 (3.2)

$$\left(\frac{m^3}{s}\right) \cdot \left(\frac{kg}{m^3}\right) = \left(\frac{kg}{s}\right)$$

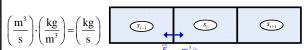


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(ii) Dispersion

- Mass change due to diffusion and mixing;
- Transport directly proportional to mass conc difference between two adjacent segments;
- Exchange of mass between segment i and segment i-1 due to dispersion:

$$+\overline{E}_{i-1,i}\cdot\left(s_{i-1}-s_{i}\right) \tag{3.3}$$



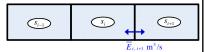


(ii) Dispersion

• Exchange of mass between segment i and segment i + 1 due to dispersion:

$$+\overline{E}_{i, i+1} \cdot (s_{i+1} - s_i)$$

$$\left(\frac{m^3}{s}\right) \cdot \left(\frac{kg}{m^3}\right) = \left(\frac{kg}{s}\right)$$



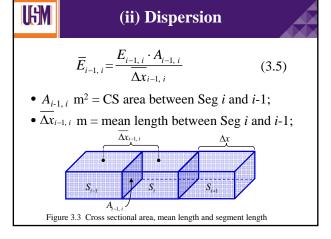
(3.4)

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(ii) Dispersion

- $S_{i-1} > S_i$: mass from Seg i-1 to i;
- $S_i > S_{i-1}$: mass from Seg i to i-1;
- Similarly for interface of Seg i and i+1;
- Bulk dispersion coefficient \overline{E} is related to E:

$$\overline{E}_{i-1, i} = \frac{E_{i-1, i} \cdot A_{i-1, i}}{\Delta x_{i-1, i}}$$
(3.5)



USM

(iii) Decay

• For mass loss due to first-order decay process:

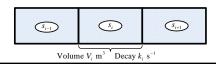
(3.6)

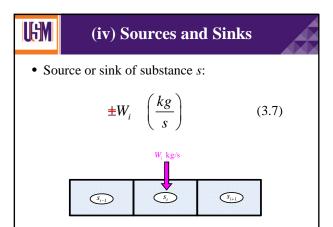
$$-k_{i} \quad V_{i} \quad s_{i}$$

$$\left(\frac{1}{s}\right) \cdot \left(m^{3}\right) \cdot \left(\frac{kg}{m^{3}}\right) = \left(\frac{kg}{s}\right)$$

with k_i s⁻¹ = decay coefficient of segment i.

 V_i m³ = volume of segment *i*.





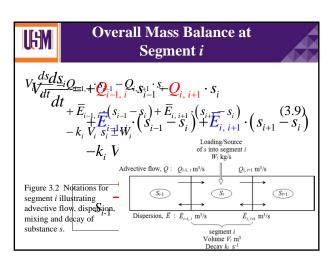
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3.2 Finite Segment Method

- Total quantity of all masses obtained must;
- = Rate of change in mass at segment i;

$$\frac{dM_i}{dt} = \frac{d(V_i s_i)}{dt} \approx V_i \frac{ds_i}{dt}$$
 (3.8)

- for $M_i = V_i$ s_i with V_i constant;
- Good approximation for most estuaries.



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3.2 Finite Segment Method

$$V_{i} \frac{ds_{i}}{dt} = Q_{i-1, i} \cdot s_{i-1} - Q_{i, i+1} \cdot s_{i}$$

$$+ \overline{E}_{i-1, i} \cdot (s_{i-1} - s_{i}) + \overline{E}_{i, i+1} \cdot (s_{i+1} - s_{i})$$

$$- k_{i} V_{i} s_{i} \pm W_{i}$$
(3.9)

• Eqn (3.9) is a numerical approx of

$$\frac{\partial s}{\partial t} = -u \frac{\partial s}{\partial x} + E \frac{\partial^2 s}{\partial x^2} - k \ s + W \tag{3.10}$$

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3.2 Finite Segment Method

- 1st order linear ODE, time-dependent;
- Assume steady-state, i.e. input, flow, exchange and reaction rate do not change with time:

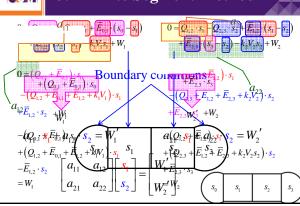
$$V_i \frac{ds_i}{dt} = 0$$
 \Rightarrow Eqn (3.9)
= linear algebraic eqn

• $n \text{ segments} \Rightarrow n \text{ number of Eqn (3.9)}.$

$$0 = Q_{i-1, i} \cdot s_{i-1} - Q_{i, i+1} \cdot s_i + \overline{E}_{i-1, i} \cdot (s_{i-1} - s_i) + \overline{E}_{i-1, i} \cdot (s_{i+1} - s_i) - k_i V_i s_i \pm W_i$$



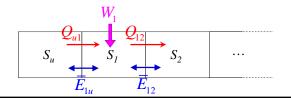
3.2 Finite Segment Method





3.2 Finite Segment Method

Segment 1:
$$0 = Q_{u1}s_u - Q_{12}s_1 + \overline{E}_{1u}(s_u - s_1) + \overline{E}_{12}(s_2 - s_1) - k_1V_1s_1 \pm W_1$$
 (3.11)

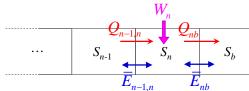


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3.2 Finite Segment Method

Segment
$$n: 0 = Q_{n-1,n} s_{n-1} - Q_{nb} s_n$$

 $+ \overline{E}_{n-1,n} (s_{n-1} - s_n) + \overline{E}_{nb} (s_b - s_n)$
 $- k_n V_n s_n \pm W_n$ (3.12)



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3.2 Finite Segment Method

$$\begin{split} \mathbf{0} &= Q_{i-1,\;i} \cdot s_{i-1} - Q_{i,\;i+1} \cdot s_i + \overline{E}_{i-1,\;i} \cdot \left(s_{i-1} - s_i \right) \\ &+ \overline{E}_{i,\;i+1} \cdot \left(s_{i+1} - s_i \right) - k_i \; V_i \; s_i \pm W_i \end{split}$$

• Group to the left all terms with s_{i-1} , s_i , s_{i+1} ;

$$(-Q_{i-1, i} - \overline{E}_{i-1, i}) \cdot s_{i-1}$$

$$+ (Q_{i, i+1} + \overline{E}_{i-1, i} + \overline{E}_{i, i+1} + k_i V_i) s_i$$

$$+ (-\overline{E}_{i, i+1}) s_{i+1} = W_i$$
(3.13)

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3.2 Finite Segment Method

Let:

$$a_{i,i-1} = -Q_{i-1, i} - \overline{E}_{i-1, i}$$
 (3.14)

$$a_{i,i} = Q_{i, i+1} + \overline{E}_{i-1, i} + \overline{E}_{i, i+1} + k_i V_i \quad (3.15)$$

$$a_{i,i+1} = -\overline{E}_{i,i+1} \tag{3.16}$$

Eqn (3.13) can be simplified to

$$a_{i,i-1} s_{i-1} + a_{i,i} s_i + a_{i,i+1} s_{i+1} = W_i$$
 (3.17)

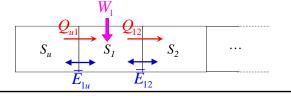
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3.2 Finite Segment Method

Segment 1:
$$Q_{1\overline{1}} s Q_{11} s_{12} s_2 Q_{12} s_1$$

= $W_1 + \overline{E} Q_{u} (s_{u} + \overline{E}_{11}) s_{\overline{u}} \overline{E}_1 V (s_2 + 3s_1^1)$

$$W_{1}' = W_{1} + Q_{u_{1}} k_{1} V_{+} S_{u_{1}} E_{1u}^{+} V_{u_{1}}$$
(83119)



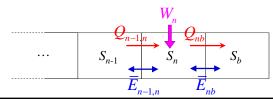
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3.2 Finite Segment Method

Segment $n: Q_{\overline{n,n}}Q_{n-R,\overline{n}1} + q_{\overline{n,n}}Q_{nb}s_n$

$$=W_{h}^{\perp}\,\overline{E}_{n}\overline{E}_{lnb}\left(s_{ln}^{-}\overline{-}W_{s_{ln}}^{\prime}\right)+\overline{E}_{nb}\left(s_{l}^{\prime}3.20_{l}\right)$$

$$W_{n} = W_{n}^{-} + E_{nb}^{-} s_{ns} + W_{n}^{-}$$
 ((3..22))



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3.2 Finite Segment Method

 \therefore The complete set of eqns for *n* segments:

(3.22)

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3.2 Finite Segment Method

In matrix form: [A](s) = (W)

$$\begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & \cdots & 0 \\ a_{21} & a_{22} & a_{23} & 0 & \cdots & \cdots & 0 \\ 0 & a_{32} & a_{33} & a_{34} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & a_{n,n-1} & a_{n,n} \end{bmatrix} \begin{pmatrix} s_1 \\ s_2 \\ s_3 \\ \vdots \\ s_n \end{pmatrix} = \begin{pmatrix} W_1' \\ W_2' \\ W_3' \\ \vdots \\ W_n' \end{pmatrix}$$

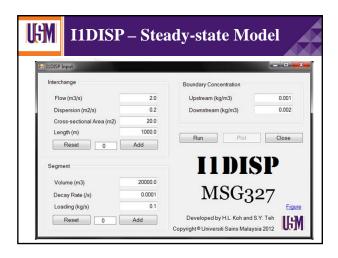
$$(m3/s) \cdot (kg/m3) = (kg/s)$$
 (3.23)

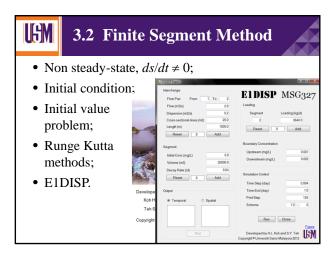
$$[A] = \text{matrix } n \times n$$
 (s) and $(W) = n \times 1 \text{ vectors}$

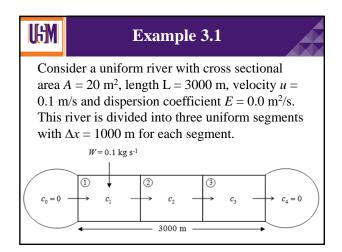
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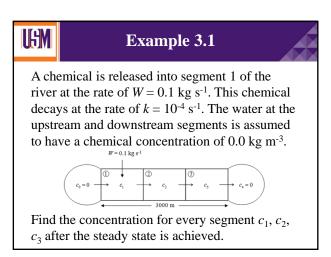
3.2 Finite Segment Method

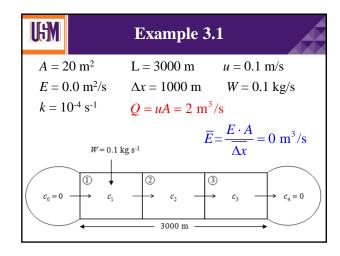
- (3.23): Boundary value problem-steady-state;
- Boundary conditions: s_u and s_b ;
- FSM can only be solved easily by hand;
- For systems of dimension 3 by 3;
- River pollution complex matter;
- Requires division of river into many segments;
- For more accurate and reliable solution.
- \Rightarrow system of equations with high dimensions;
- Numerical method I1DISP (Koh, 2004).

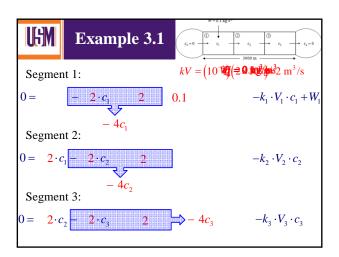


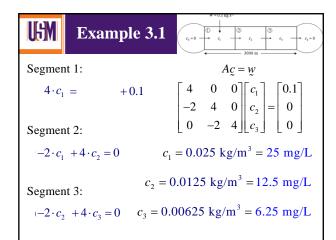


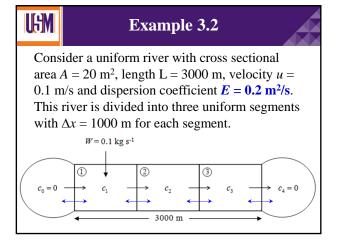












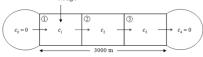
A chemical is released into segment 1 of the decays at the rate of $k = 10^{-4}$ s⁻¹. The water at the

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river at the rate of $W = 0.1 \text{ kg s}^{-1}$. This chemical upstream and downstream segments is assumed to have a chemical concentration of 0.0 kg m⁻³.

Example 3.2



Find the concentration for every segment c_1 , c_2 , c_3 after the steady state is achieved.

USM Example 3.2 $A = 20 \text{ m}^2$ L = 3000 mu = 0.1 m/s $E = 0.2 \text{ m}^2/\text{s}$ $\Delta x = 1000 \text{ m}$ W = 0.1 kg/s $k = 10^{-4} \text{ s}^{-1}$ $Q = uA = 2 \text{ m}^3/\text{s}$ $\overline{E} = \frac{E \cdot A}{\overline{\Delta x}} = 0.004 \text{ m}^3/\text{s}$ $W = 0.1 \text{ kg s}^{-1}$ 3000 m

Example 3.2 - Solution $A\underline{s} = \begin{pmatrix} 4.008 & -0.004 & 0 \\ -2.004 & 4.008 & -0.004 \\ 0 & -2.004 & 4.008 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0.1 \\ 0 \\ 0 \end{pmatrix} = \underline{w}$ $c_1 = 0.02496 \text{ kg/m}^3$ or $c_1 = 24.96 \text{ mg/L}$ $c_2 = 0.01249 \text{ kg/m}^3$ or $c_2 = 12.49 \text{ mg/L}$ $c_3 = 0.00624 \text{ kg/m}^3$ or $c_3 = 6.24 \text{ mg/L}$

