LECTURE

MODELLING THE MARINE ENVIRONMENT

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Lecture 7

THE SUBSTANCE TRANSMISSION PROCESS

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Lecture 7C

CALCULATION METHODOLOGY PROFICIENT FUSION SYSTEMS

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CONTENT

- **Euler Method**
- **Heun Method**
- **Runge-Kutt Method**

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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.*

Euler Method

The complete mixed lake model

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

where

$$\lambda = \frac{Q}{V} + k + \frac{v}{H} \qquad (2)$$

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

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

Substituting (3) into the equation (1):

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

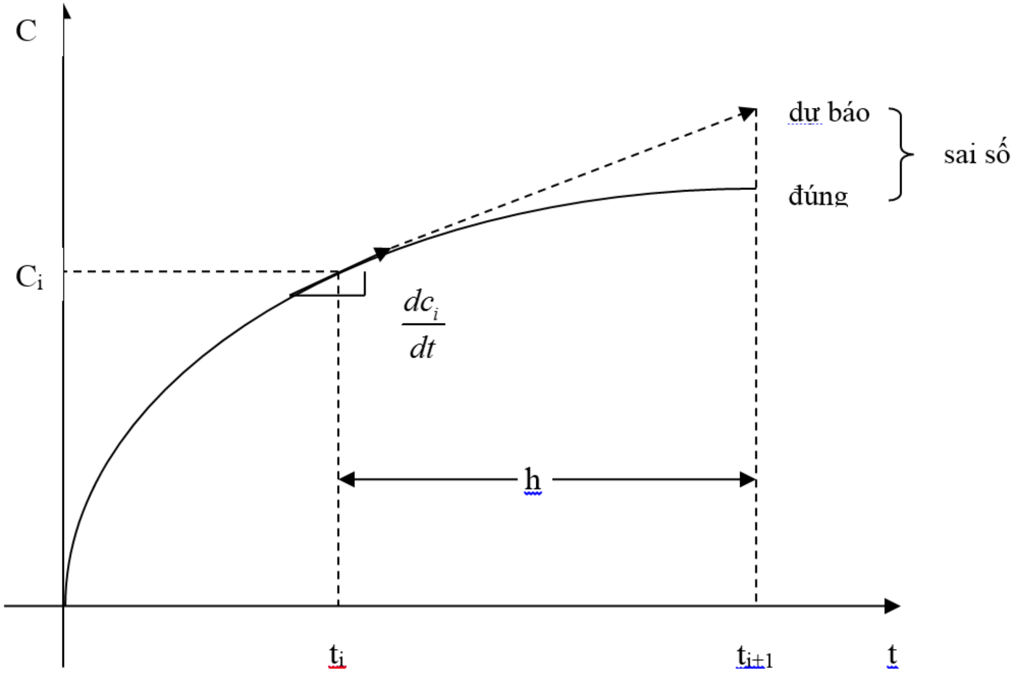
Euler Method

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

This method can be generalized as follows:

$$C_{i+1} = C_i + f(t_i, C_i) h \qquad (6)$$

Where $f(t_i,C_i) = dC_i/dt$ Tthe value calculated at t_i và C_i, và $h = t_{i+1} - t_i$.



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

At t = 0, the lake receives a loading of 50×10^6 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:

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

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Solution

(a) Eigenvalue is calculated as follows

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

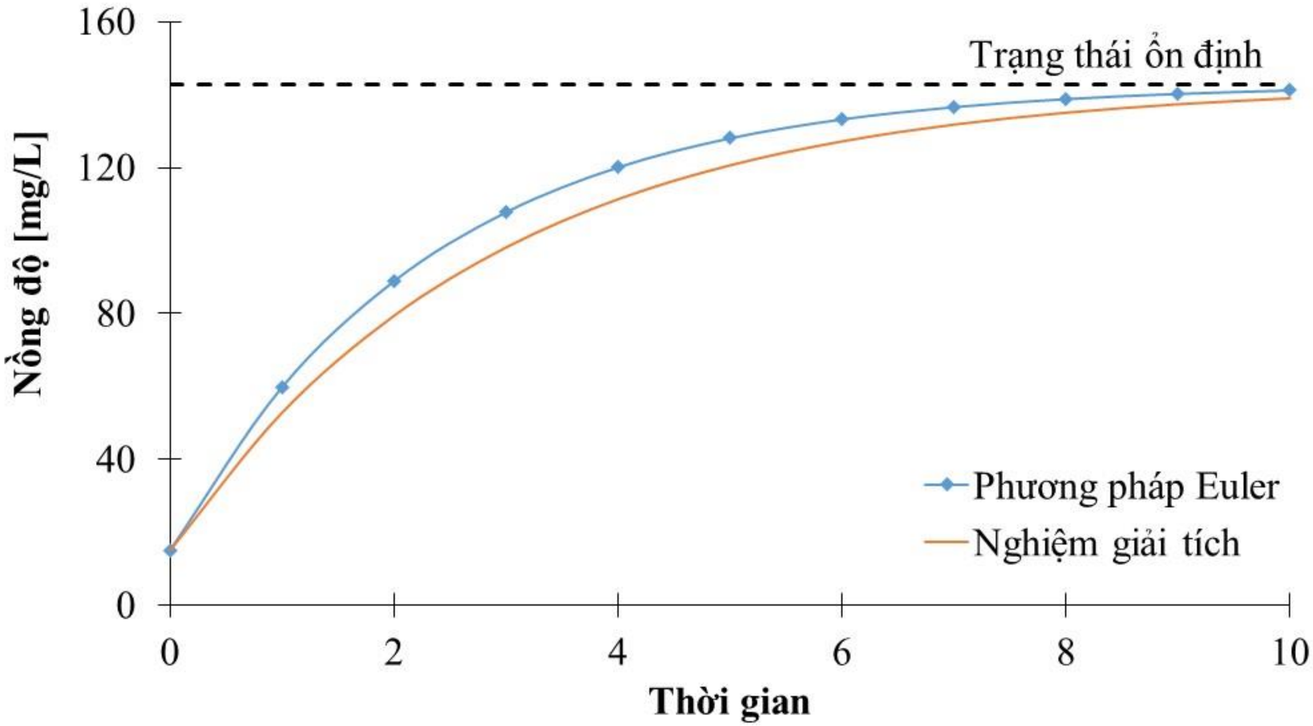
At the beginning (t =0), the concentration of the lake is 15 mg/L and receive a loading is $50x10^6$ g/yr.

At t=1 year

$$C(1) = 15 + \left[\frac{50\times10^6}{10^6} - 0.35(15)\right]\times1.0 = 59.75(mg/l)$$

At t=2 year

$$C(2) = 59.75 + \left[\frac{50\times10^6}{10^6} - 0.35(59.75)\right]\times1.0 = 88.8375(mg/l)$$



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Graph comparing the euler method solution and the analytical solution

t (yr)	C (mg/L)		t (yr)	C (mg/L)	
	PP Euler	Analytical method		PP Euler	Analytical 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	∞	142.86	142.86

HEUN METHOD

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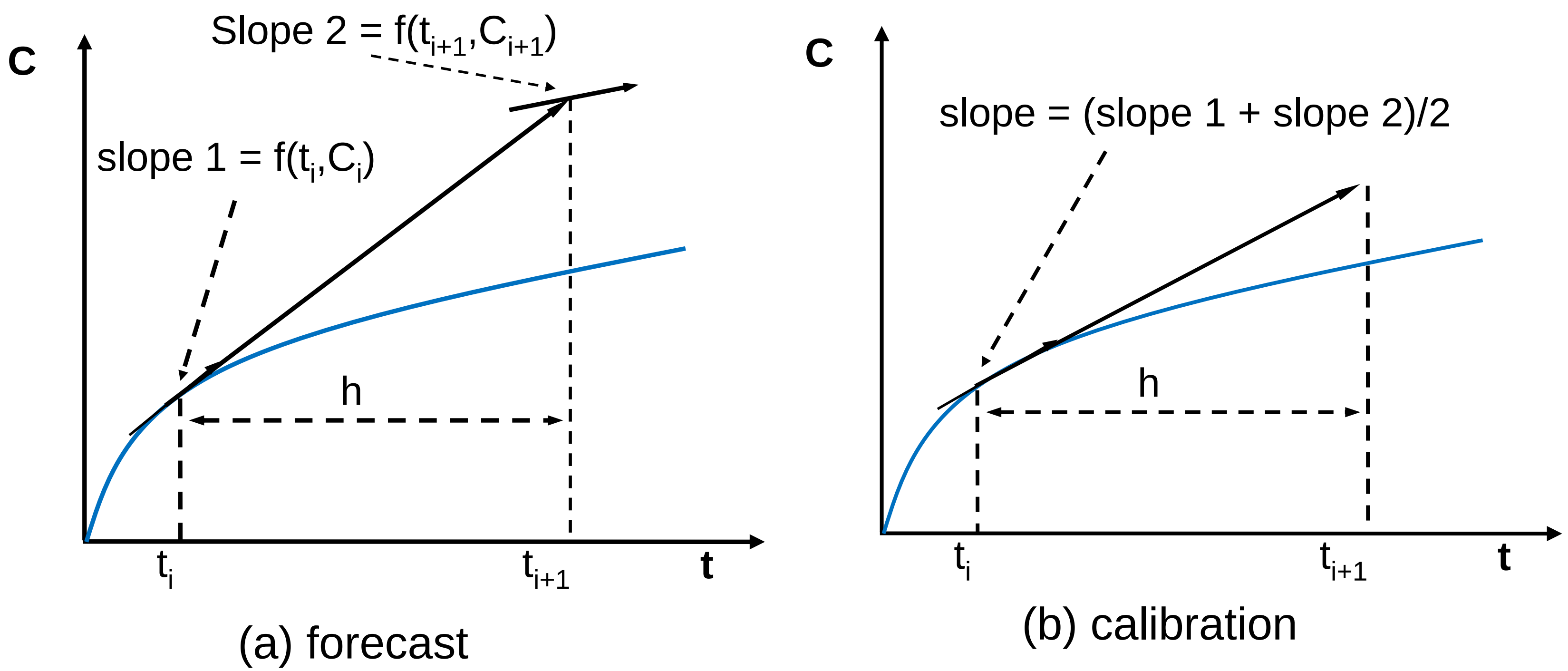
One method to improve the error in the Euler method is to identify the derivative on either side of a time step - one at the beginning (t_i) and one at the end (t_{i+1}). These two derivative components are then taken on average to estimate the slope of the entire time step (h)



Graphical describing the Heun method

HEUN METHOD

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

Forecast:

$$C_{i+1}^{0} = C_i + f\left(t_i, C_i\right)h \quad (7)$$

Calibratation *h:*

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

Example 2. A well-mixed lake has the following characteristics: Q = 10^5 m^3/yr, V = 10^6 m^3, 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 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 :

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

Solution

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(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 50×10^6 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

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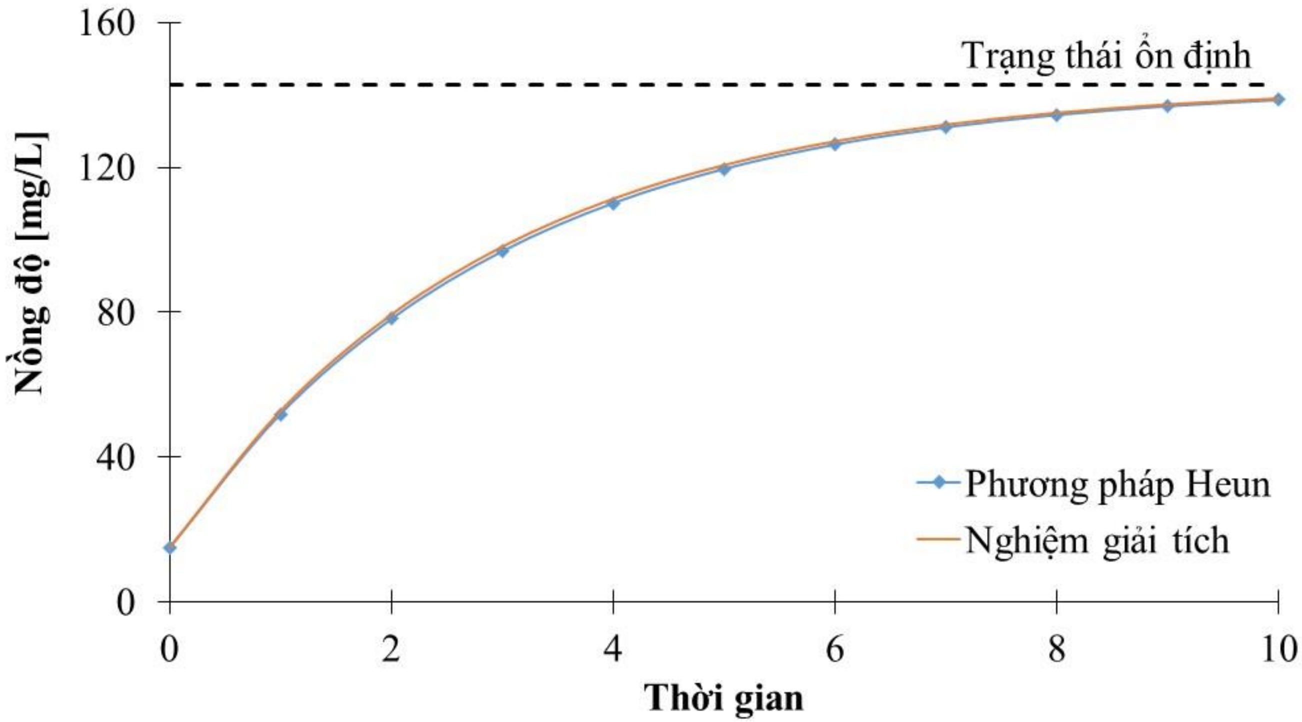

Graph comparing the solution by the Heun method and the Analytical solution

t (yr)	C (mg/L)		t (yr)	C (mg/L)	
	PP Heun	Analytical method		PP Heun	Analytical 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	∞	142.86	142.86

Runge-Kutta Method

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

ϕ 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:

$$C_{i+1} = C_i + \left[\frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)\right]h \quad (10)$$

Where

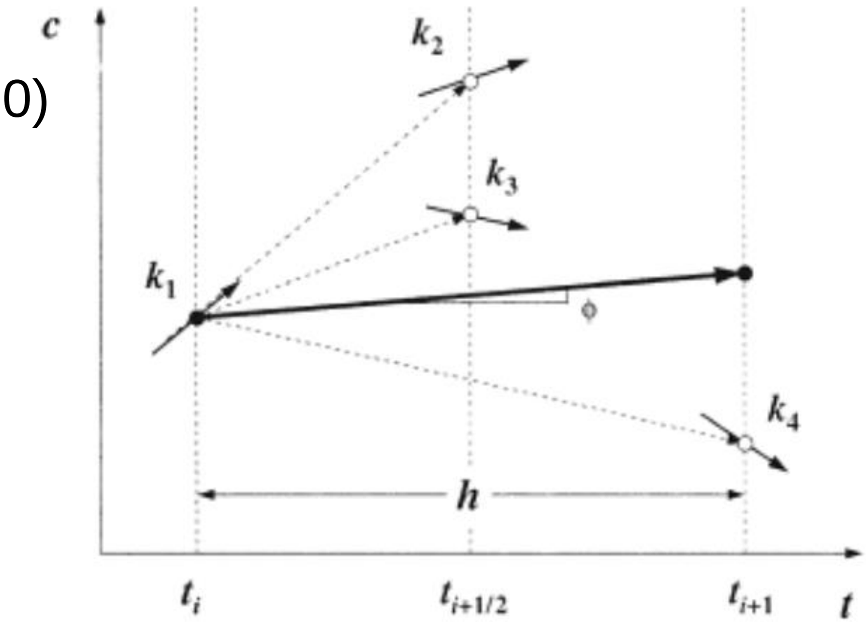
$$k_1 = f\left(t_i, C_i\right)$$

$$k_2 = f\left(t_i + \frac{1}{2}h, C_i + \frac{1}{2}hk_1\right)$$

$$k_3 = f\left(t_i + \frac{1}{2}h, C_i + \frac{1}{2}hk_2\right)$$

$$k_4 = f\left(t_i + h, C_i + hk_3\right)$$

$$f\left(t, C\right) = \frac{dC}{dt}\left(t, C\right)$$



Graph describing the Rungge-Kutta method

Runge-Kutta Method

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

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

where

$$k_1 = f\left(t_i, C_i\right)$$

$$k_2 = f\left(t_i + \frac{1}{4}h, C_i + \frac{1}{4}hk_1\right)$$

$$k_3 = f\left(t_i + \frac{1}{4}h, C_i + \frac{1}{8}hk_1 + \frac{1}{8}hk_2\right)$$

$$k_4 = f\left(t_i + \frac{1}{2}h, C_i - \frac{1}{2}hk_2 + hk_3\right)$$

$$k_5 = f\left(t_i + \frac{3}{4}h, C_i + \frac{3}{16}hk_1 + \frac{9}{16}hk_4\right)$$

$$k_6 = f\left(t_i + h, C_i - \frac{3}{7}hk_1 + \frac{2}{7}hk_2 + \frac{12}{7}hk_3 - \frac{12}{7}hk_4 + \frac{8}{7}hk_5\right)$$

Example 3. A well-mixed lake has the following characteristics: Q = 10^5 m^3/yr, V = 10^6 m^3, 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 :

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

System equations

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

$$\frac{dC_1}{dt} = f_1(C_1, C_2, \ldots, C_n) \quad (12)$$

$$\frac{dC_2}{dt} = f_2(C_1, C_2, \ldots, C_n) \quad (13)$$

$$\frac{dC_n}{dt} = f_n(C_1, C_2, \ldots, C_n) \quad (14)$$

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

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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^3)	0.5×10^6	0.6×10^6
Output (m^3/yr)	1×10^6	1×10^6

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.