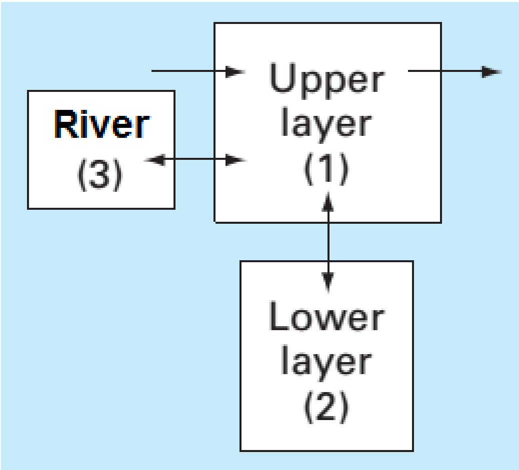
River and Stratified lake problem

You have been contacted as an engineer by a Water Board due to a common problem in a confidential location of a River-Lake system in The Netherlands. The water board is interested in estimating the mixing that occurs between a stratified lake (upper layer and lower layer) with respect to an adjacent river (Figure 1).

Figure 1 - System of River and stratified lake (Upper layer and Lower layer).



After getting the contract you have performed a tracer campaign in the system using a conservative tracer which is instantaneously mixed with the river water. Afterwards the tracer concentration is monitored over the ensuing period (20 days) in all three locations. You obtained the values presented in Table 1.

Table 1 - Measurements in the three areas

t	C_1	C_2	C_3
[d]	[mg/l]	[mg/l]	[mg/l]
0	0	0	100
2	15	3	48
4	11	5	26
6	7	7	16
8	6	7	10
12	3	6	4
16	2	4	3
20	1	2	2

Solution

Using mass balances, the system can be modeled as the following simultaneous Ordinary Differential Equations (ODE's) of Equation 1.

Equation 1 - System of equations in the river lake system

$$V_1 \frac{dC_1}{dt} = -Q \cdot C_1 + E_{12} \cdot (C_2 - C_1) + E_{13} \cdot (C_3 - C_1)$$
$$V_2 \frac{dC_2}{dt} = E_{12} \cdot (C_1 - C_2)$$
$$V_3 \frac{dC_3}{dt} = E_{13} \cdot (C_1 - C_3)$$

Where $V_i =$ volume of segment i, $Q =$ flow, and $E_{ij} =$ diffusive mixing rate between segments i and j.

You are going to estimate the ***E's***, if $V_1 = 1 \times 10^7$, $V_2 = 8 \times 10^6$, $V_3 = 5 \times 10^6$, and $Q = 4 \times 10^6$, which minimizes the total Sum of Squared Residuals (SSR_{TOTAL}).

Equation 2 - Calculation of total SSR.

$$err = (C_{measured} - C_{predicted})$$
$$SSR_t = err^2$$
$$SSR_{TOTAL} = \sum_{t=0}^{20} SSR_t$$

Notice that *err* can be either positive or negative, while SSR_{TOTAL} is only positive (Equation 2).

Second, you need to model the behavior of the system using the ODE's (Equation 1). For this purpose an executable which solves the Equation 1, and estimates concentrations of the 3 components (1 river and 2 layers in the lake) at the measured time steps as in Table 1 (column 1) is provided. In addition, the executable creates a figure of the behavior of the system in time and also provides a results file which presents the calculations made.

The problem is to identify the combination of parameters E_{12} and E_{13}, which minimizes *SSR*.

1) Run the executable "***.exe***"
2) If you are not able to make it run. It is because you do not have the required MATLAB license. You will need to download the corresponding MATLAB Compiler Runtime (MCR) for your particular PC or laptop. It is dependent on the corresponding version of your Operative System (OS) for *Windows*, *Linux* or *Mac*. You may find the required MCR files in the following website:

   http://www.mathworks.nl/products/compiler/mcr/

   Please download the one corresponding to your OS. And follow the instructions presented in the website.
3) Run the executable "***.exe***"

4) Leave the parameters E_{12} and E_{13}, as they are currently set. You must obtain a result similar to Figure 2.

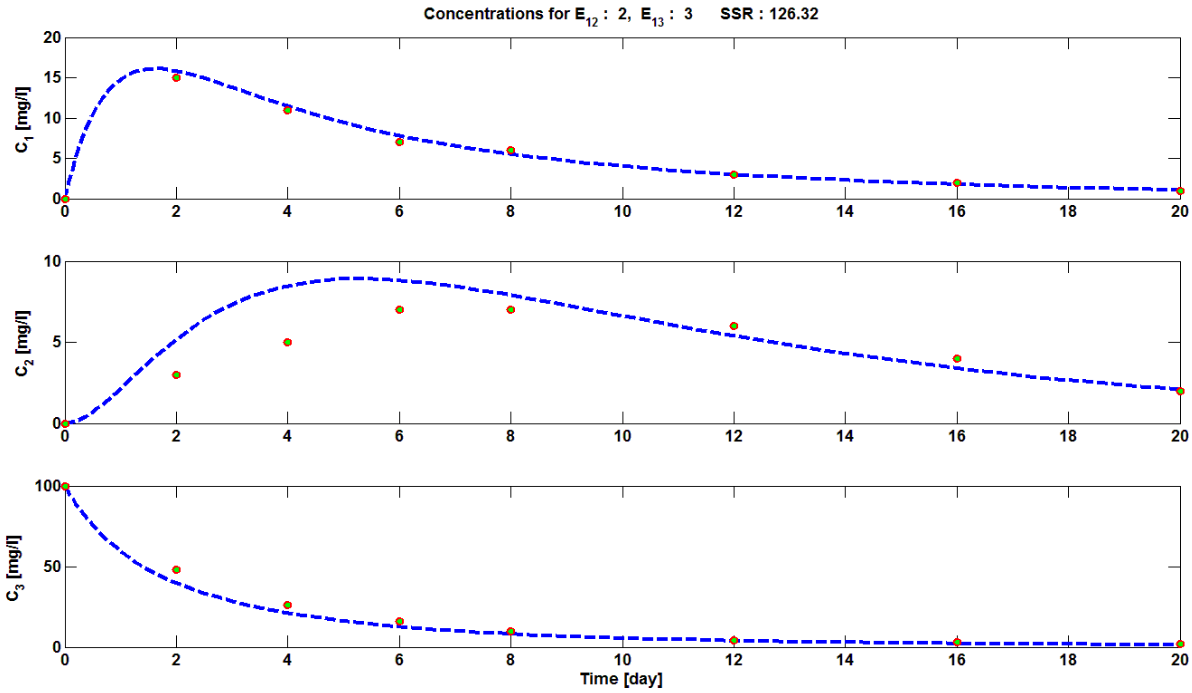


Figure 2 - Results of simulation with E_{12} = 2.0 and E_{13} = 3.0.

Notice that the behavior of the upper layer of the lake (C_1) is very similar to the behavior of the measured data. Even the concentrations on the river (C_3) are very similar in shape to the ones obtained in the measurement campaign. On the other hand the behavior of the lower layer (C_2) follows the trend of the measured data, but the estimated values are higher than the measured ones.

5) Open the data stored in the file of the results "***.dat***". You may find that the results are like the ones below. In the lower part where the SSR are stored, it has been highlighted the maximum values for each part of the system.
Surprisingly the highest error occurs for the river concentration (C_3) during day 2 with an SSR of 66.890. This shows that visual adjustment can be misleading.

Table 2 - Typical results file obtained after running the simulation.

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River and stratified lake problem
Solution with:
  E12      E13
2.000   3.000

Measured Data
 Day      C1     C2     C3
00      0.000        0.000        100.000
02      15.000       3.000        48.000
04      11.000       5.000        26.000
06      7.000        7.000        16.000
08      6.000        7.000        10.000
12      3.000        6.000        4.000
16      2.000        4.000        3.000
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20      1.000        2.000        2.000
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Predicted Data
 Day     C1     C2     C3
00      0.000        0.000        100.000
02      15.850       5.176        39.821
04      11.455       8.478        21.307
06      7.825        8.820        12.824
08      5.537        7.907        8.318
12      3.040        5.394        4.113
16      1.781        3.404        2.304
20      1.069        2.096        1.360
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Squares of Residuals
 Day     C1     C2     C3
00      0.000        0.000        0.000
02      0.722        4.733        66.890
04      0.207        12.099       22.025
06      0.680        3.314        10.090
08      0.214        0.822        2.830
12      0.002        0.367        0.013
16      0.048        0.355        0.484
20      0.005        0.009        0.410
   ------------------------
        1.878        21.699       102.741
                                 126.318
```

6) Now your task is to use the executable by changing the parameters E_{12} and E_{13}, until reaching a minimum value of ***SSR***. For this prepare an Excel table in which you may be able to identify the range of E_{12} and E_{13} which makes ***SSR*** reach a minimum (Table 3).

Table 3 - Initial range of parameters.

		E_{12}								
		1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
E_{13}	1.0									
	1.5									
	2.0									
	2.5									
	3.0									
	3.5									
	4.0									
	4.5									
	5.0									

Now that you have identified a range of values, find which combination of E_{12} and E_{13} makes ***SSR*** reach a minimum. Present your results in Table 4.

Table 4 - Obtained results by variation of the parameters.

		E_{12}				
E_{13}						
