

# BT5240 - Assignment 3

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1)

NOTE: Parameter vector is denoted as  $V = [Vm_1 \ Vm_2 \ Vm_3 \ Vm_4]$

Methodology:

For a given  $V$ , we solve the set of ODEs and return the simulation results (or we can call it predictions). These predictions are compared with the true values present in *data.csv* and an objective function is designed which captures the deviation (error) of predictions from true values. The last step is to perform a search in the parameter space (in this case, the parameter is  $V$ ) and find the set of parameters which minimize the objective function.

Objective function:  $L2 - norm$  (Frobenius norm) of the error matrix.

Optimization is carried out using *fminsearch* routine in *MATLAB*.

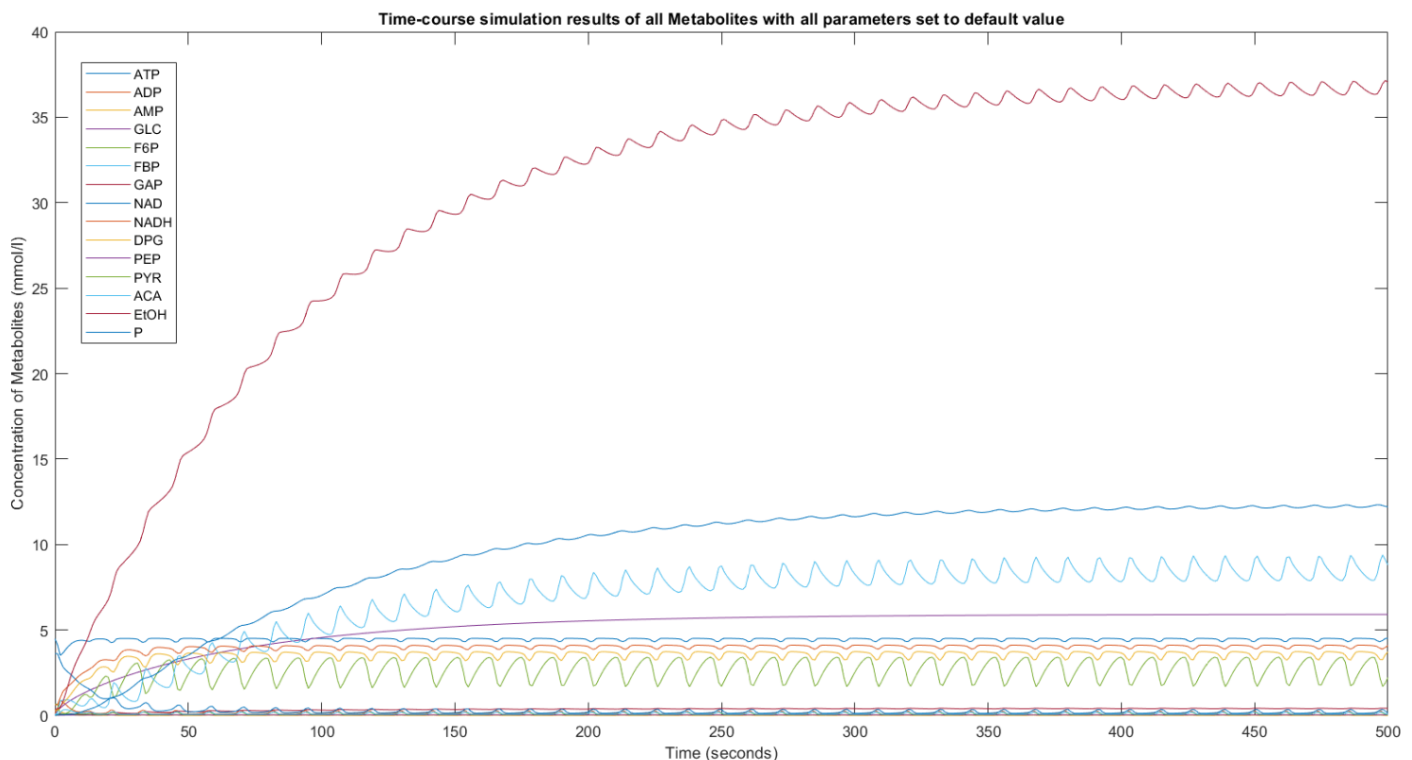
The result is attached below:

Estimated  $Vm$  after minimizing the objective function:

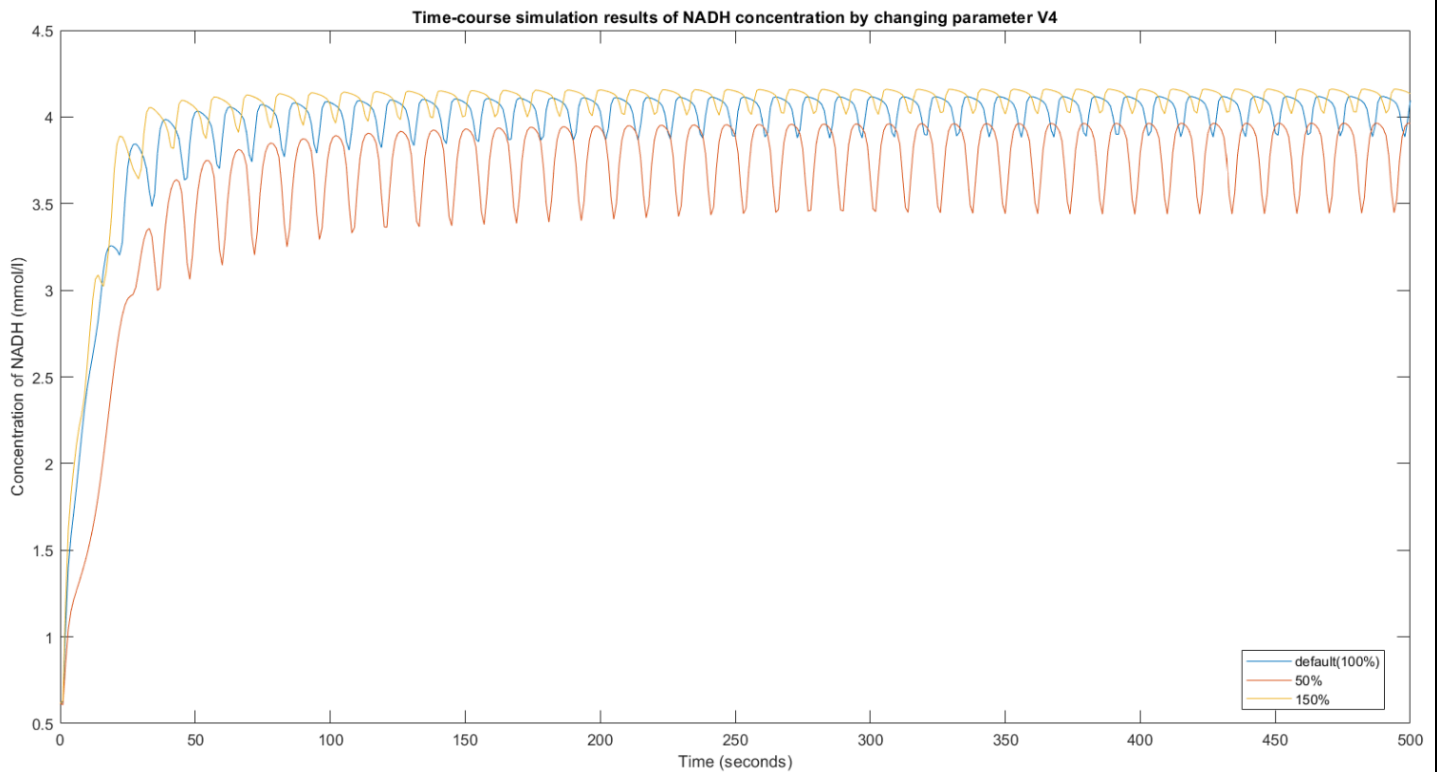
```
--> Vm1 = 5.848137  
--> Vm2 = 201.656490  
--> Vm3 = 4.412595  
--> Vm4 = 5.881587
```

2.i)

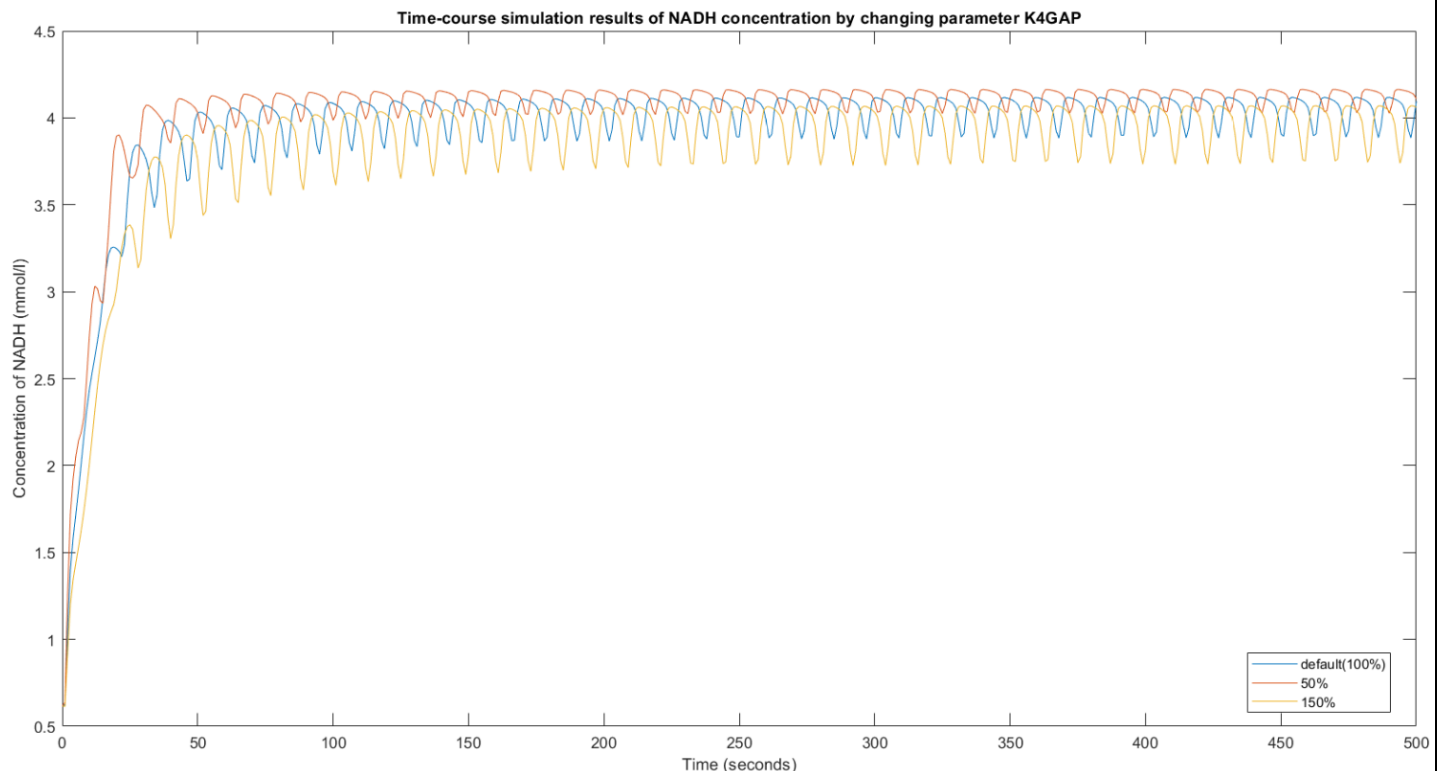
The set of ODEs are solved using *ode23* routine in *MATLAB*.



## 2.ii)

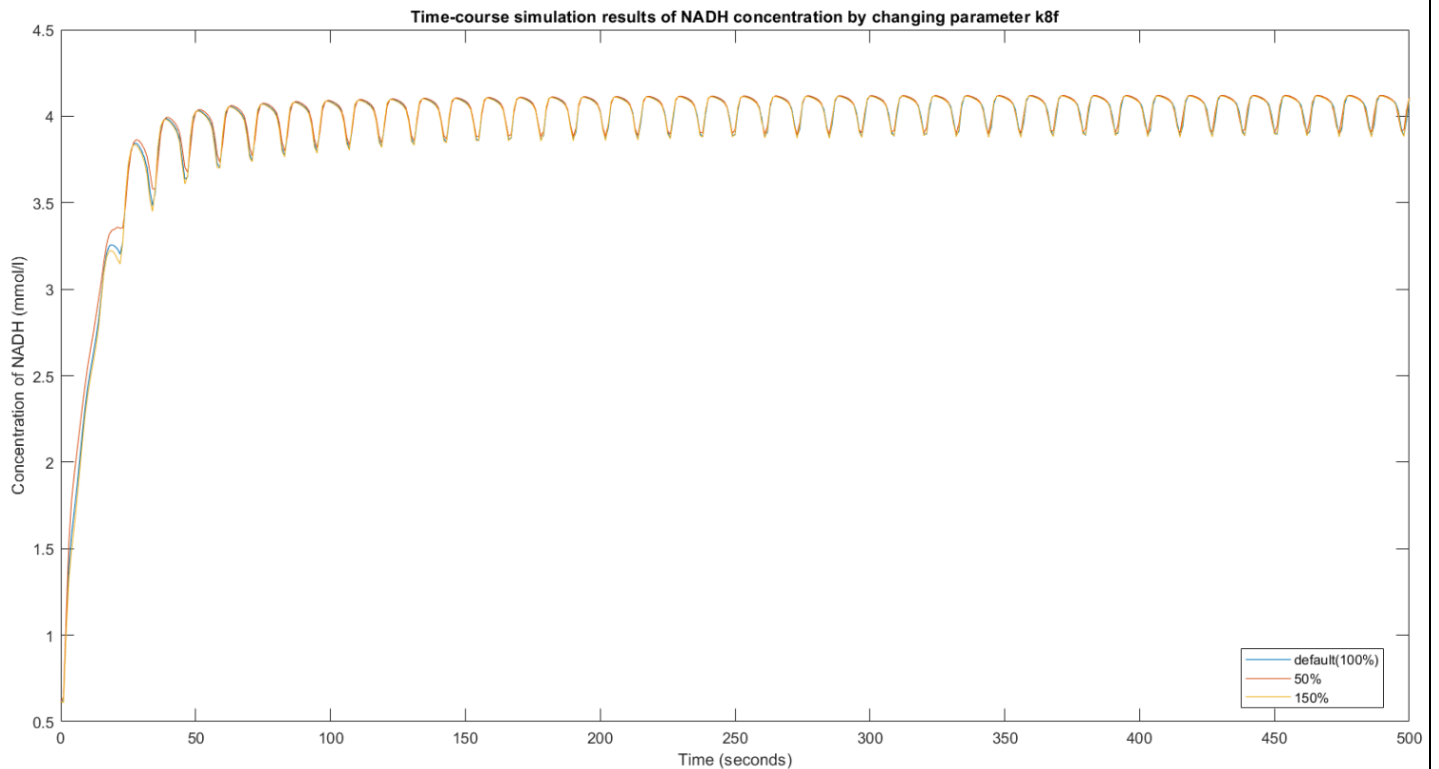


From the above plot we can infer that by changing  $V_4$  to 50 % of its original value, the average concentration of  $NADH$  decreases when compared to the original. On the other hand, by changing  $V_4$  to 150 % of the default value, the average concentration of  $NADH$  slightly increases when compared to the original. This shows that there is a small positive correlation between value of parameter  $V_4$  and concentration of  $NADH$ .

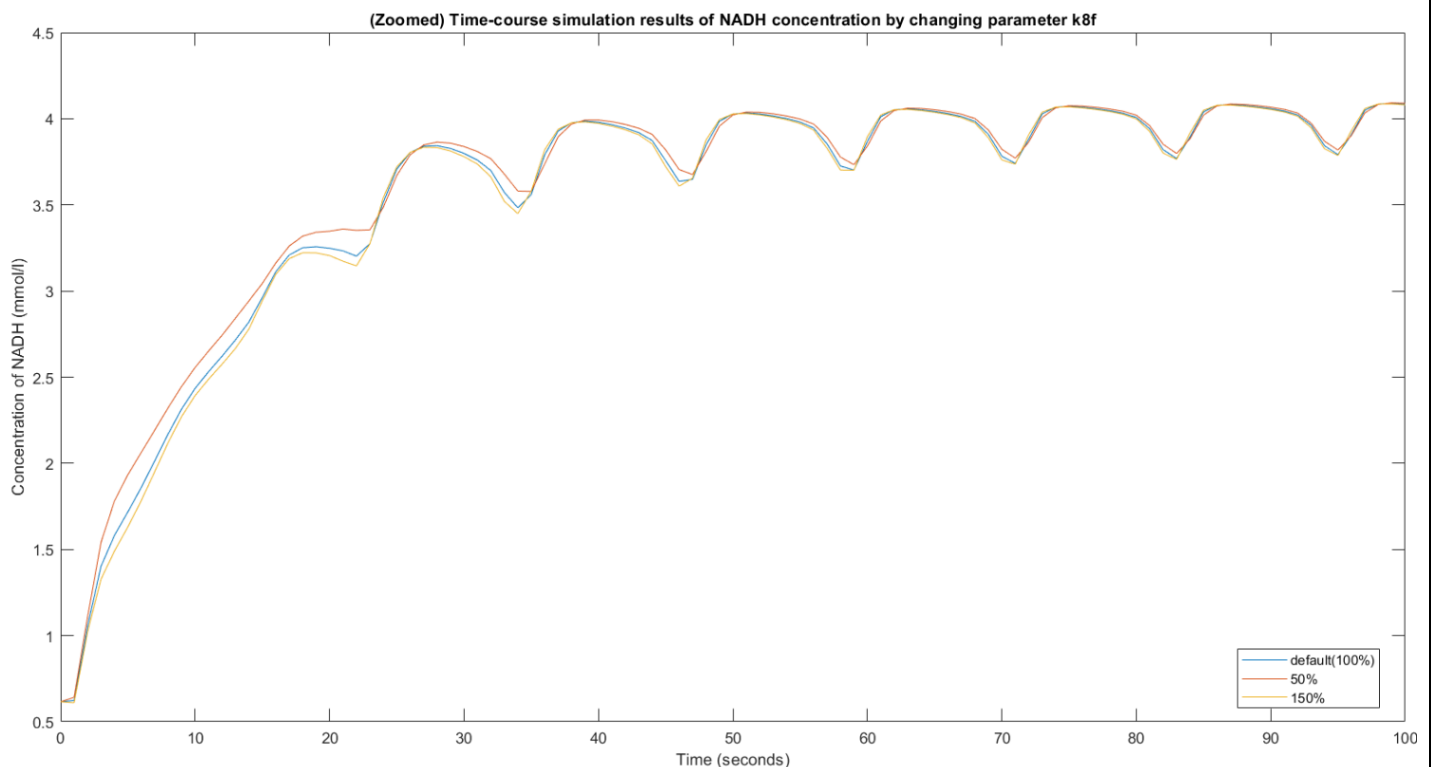


From the above plot we can infer that by changing  $K_4GAP$  to 150 % of its original value, the average concentration of  $NADH$  slightly decreases when compared to

the original. On the other hand, by changing  $K4GAP$  to 50 % of the default value, the average concentration of  $NADH$  slightly increases when compared to the original. This shows that there is a small negative correlation between value of parameter  $K4GAP$  and concentration of  $NADH$ .

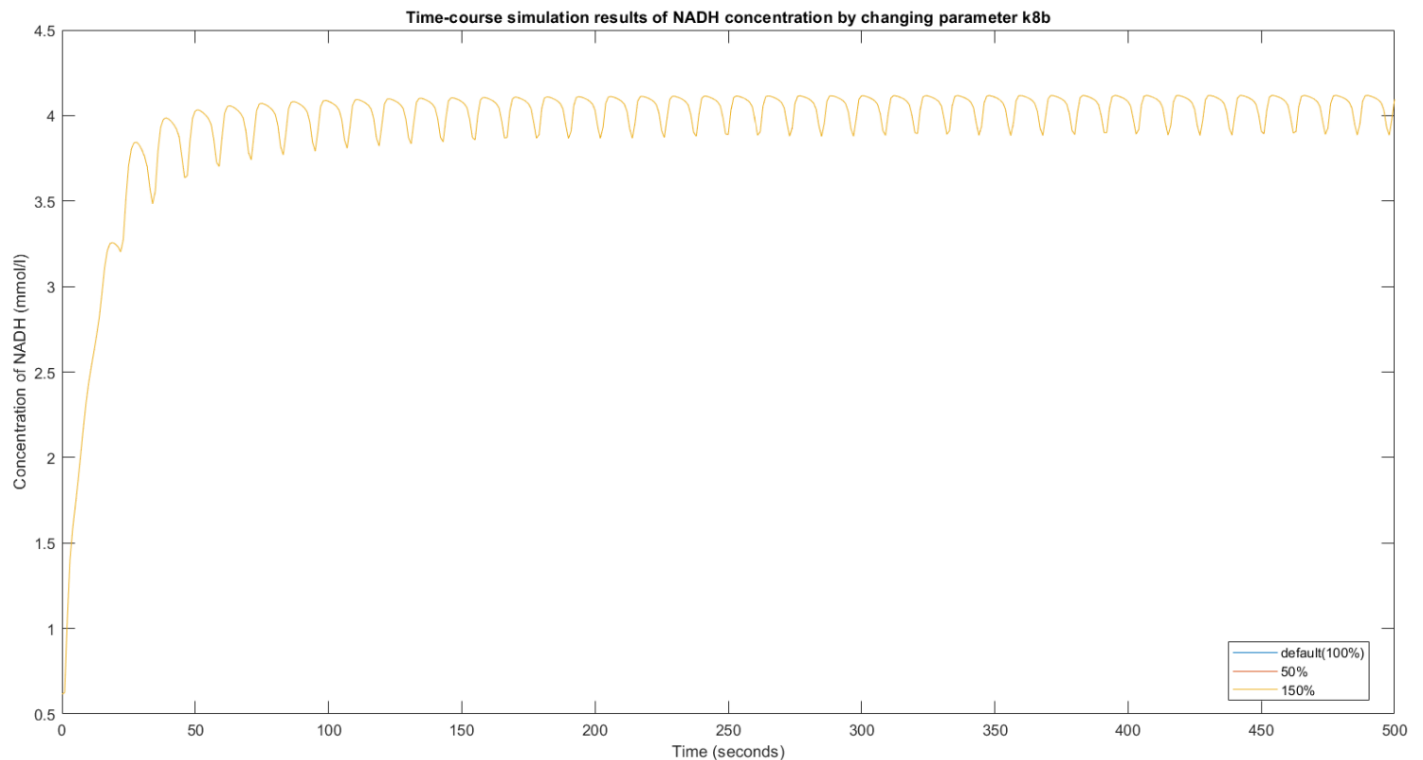


From the above plot, we can see that change in  $k8f$  influences the concentration of  $NADH$  only in the initial period of time. Let us zoom into that window and observe the effects.



As we can see from the above zoomed plot, when  $k8f$  is reduced to 50 % of its original value, the concentration of  $NADH$  has slightly increased during 0 to 70

seconds and then eventually merges with the concentration curve of *NADH* corresponding to default value of *NADH*. On the other hand, when  $k8f$  is increased to 150 % of its original value, we can observe a very minute decrease in the corresponding concentration curve as compared to that corresponding to default value of  $k8f$  in the window between 0 to 70 seconds. The curve corresponding to 150 % also merges with the curve corresponding to default value of  $k8f$  beyond 70 seconds.



From the above plot, we can see that all the three curves overlap perfectly. This implies that change in  $k8b$  has no effect in the concentration of *NADH*.

#### Summary of the study:

Parameter	Influence on average concentration of <i>NADH</i>
$V4$	slight positive correlation
$K4GAP$	slight negative correlation
$k8f$	slight negative correlation only during the initial phase of simulation (between 0 to 70 seconds)
$k8b$	no correlation/influence

#### Code files

Main codes: *q1\_files/q1.m*, *q2\_files/q2.m* for question 1 and question 2

All other *.m* files in *q2\_files* directory are auxiliary codes which are used by *q2.m*