

Additional materials for the article

Lashin S.A., Klimenko A.I., Mustafin Z.S., Kolchanov N.A., Matushkin Yu.G. published in “*Matematicheskaya biologiya i bioinformatika*”. 2014. V. 9. № 2. P. 585–596. URL: http://www.matbio.org/2014/Lashin_9_585.pdf.

MANUAL DESCRIBING THE CREATION OF “POISONER-PREY” MODEL

How to create the “poisoner-prey” model using the HEC GUI

An example of “poisoner-prey” model was previously described in [16]. In order to create this model using the HEC GUI one should follow the instructions.

1. Go to menu: “File” → ”New model”.
2. Set the "Environmental volume" value to $1e-2$ and "Environmental flow" to $2e-2$.
3. In the group "Nonspecific substrates" set the "Initial concentrations" for the substrate "1:" to $1e-5$, and the "Inflow concentrations" to $5e-2$.
4. To set the number of specific substrates, change the “Quantity” value ("Specific substrates" group) to 2.
5. Set the initial concentrations for specific substrates (S1 and S2) to $1e-5$.

Set initial poisoner population

The “Next” button opens the tab for editing of the population settings. At first, click the “Add new population” button to create the “poisoner” population.

1. In the opened window, set the “Size (number of cells)” value to $1e+5$ (100000 cells).
2. Choose the RUBEL strategy in the “Trophic strategy” combobox.
3. Set its parameters to $1e-8$ and $2e-2$ for “Death coefficient” and “Flow coefficient”, respectively.
4. Set the consumption and synthesis parameters located in the corresponding group: consumption rate parameters (for nonspecific and specific substrates) set to $1e+7$ and $1e+9$ respectively, while the synthesis rate parameter should be set to $1e+6$.
5. The following operations should be done for setting the population genome: three genes should be added – the first for N1 utilization, the second for S1 utilization, and the third one for S2 synthesis.
6. To add these genes, click the “Specific utilization” button at first. The gene addition menu will be opened.
 - a) Choose S1 in the “Substrate number” combobox, then set alleles distribution for the corresponding gene. More exactly, you should set alleles values and concentration. By default, there is only one allele for a gene in the population.
 - b) To add 9 alleles, click 9 times the button “Add allele”. Then set alleles’ values to 3, 4, 5, 6, 7, 8, 9, 10, 11, 12 using the top spinners; leave default values in the bottom spinners (alleles’ concentrations will be normalized automatically).
 - c) Press “Ok”.
7. As in the case before, add the gene for N1 utilization with the only allele (value = 3, concentration = 1).
8. As in the case before, add the gene for S2 synthesis with the only allele (value = 3, concentration = 1).
9. Press “Ok”. The poisoner population has will be added to the model.

Set initial prey population

Add the “prey” population in the similar manner. The prey parameters:

1. “Size (number of cells)”: $1e+5$
2. “Trophic strategy”: INH (inhibitory)
3. “Death coefficient”: $1e-8$
4. “Flow coefficient”: $2e-2$

5. “Consumption rate (nonspecific substrates)”: $1e+7$
 6. “Consumption rate (specific substrates)”: $7e+5$
 7. “Synthesis rate”: $1e+7$
 8. As it is done before, add three genes to the genome: first for N1 utilization, second for S2 utilization, third for S1 synthesis. First and third genes should have one allele (value = 3, concentration = 1), while the second – ten alleles (values = 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, concentrations by default).
 9. Press “Ok”. The prey population has will be added to the model.
- Finally, press the “Next” button, which opens the additional parameters tab. Leave them by default and press the “Finish” button. The model will be created.