

Welcome to EasyModel!

This tutorial will teach you how to model and simulate a systems biology model.

In each slide you will find annotations, indicating how you can use the user interface.

Press next to start the tutorial (or press skip to use EasyModel).

Model editor *Rate editor*

$$n_1 * S_1 + n_2 * S_2 + \dots \rightarrow m_1 * P_1 + m_2 * P_2 + \dots ; M_1; M_2; \dots$$

n_i, m_i : Stoichiometric coefficient.
 S_i, P_i : Substrates and Products.
 M_i : Modifiers that can activate or inhibit the reaction rate.



Species Settings

Name	Initial Concentration	Variable Type
C	0.01	Time Dependent ▾
M	0.01	Time Dependent ▾
X	0.01	Time Dependent ▾

Ok Cancel

3. Set initial concentrations and variable types

Species

Velocity Rates

4. Create or import rates

+ New Rate

Import Rates

New Rate

Rate Name
BIOMD003_K8

Rate Definition
 $\text{cell} \cdot (1 - M) \cdot (C \cdot V_{M1} \cdot (C + K_c)^{-1}) \cdot (K_1 - M + 1)$

Rate Options

☐ One substrate only
☐ No products
☐ One modifier only

Ok Cancel

Import Predefined Rates

<input type="checkbox"/>	Name	Rate Definition
<input checked="" type="checkbox"/>	Power Laws	$a \cdot X_1^{g_1} \dots X_n^{g_n}$
<input type="checkbox"/>	Saturating Cooperative	$v \cdot X_1^{g_1} \dots X_2^{g_n} / ((KX_1 + X_1)^{g_1} \dots (KX_2 + X_2)^{g_n})$
<input type="checkbox"/>	Saturating	$v \cdot X_1 \dots X_2 / ((KX_1 + X_1) \dots (KX_n + X_n))$
<input type="checkbox"/>	Mass action	$a \cdot X_1^{n_1} \dots X_2^{n_n}$
<input type="checkbox"/>	Henri-Michaelis menten	$(v \cdot b : XF) / (k + b : XF)$
<input type="checkbox"/>	Hill Cooperativity	$(v \cdot (b : XF^n)) / (k^n + b : XF^n)$
<input type="checkbox"/>	Catalytic activation	$(v \cdot b : XF \cdot b : MF) / ((k + b : XF) \cdot (k_2 + b : MF))$
<input type="checkbox"/>	Competitive inhibition	$(v \cdot b : XF \cdot b : MF) / ((k + b : XF) + (k + b : MF / k_2))$
<input type="checkbox"/>	EZM_KE_1	$k_1 \cdot x_1 \cdot x_2 / (k_2 + x_2)$

Import Cancel

Rate -> Reaction (R3)

BIOMD003_K3

Generic parameter values

Parameter	Numeric	Substrate	Modifier
C		C	
Kd	0.02		
X			X
cell	1		
vd	0.25		

Ok Cancel

5. Select a rate for each reaction and set a value for all the rate's parameters. Each parameter must have either a numeric value, a reference to a substrate, or a reference to a modifier.

Dynamic simulation: time evolution of the species in the model.

Steady state simulation: calculates the steady states (non-trivial equilibriums) of the biological system. These steady states remain constant over the time.

EASY MODEL Select Model Model **Simulation** Results Tools

Simulation configuration for BIOMD003 Goldpeter1991 - Min Mit Oscil

Simulation Type

☒ Deterministic
☐ Stochastic

Plot Settings

Run Simulation

☒ **Dynamic Simulation**

Dynamic Settings

Initial time 0
Final time 100
Time step 0.1

☒ Gains
☒ Sensitivities

☒ **Steady State Simulation**

Steady State Settings

Threshold 10⁻¹²

☒ Stability analysis
☐ Gains
☐ Sensitivities

Parameter Scan

Plot Settings

Font Size
Image Width (pixels)

☒ Font Bold
☐ Font Italic

Line Thickness

Plot settings: contains several configuration parameters for the graphical plots that will be performed.

*"Gains" option analyses how changes in the independent variables affect the values of the time-dependent variables.
"Sensitivities" option analyses how changes in the parameter values affect the values of the time-dependent variables.
"Stability analysis" calculates if the steady state (homeostasis) is stable (negative real parts for all eigenvalues) or not (non-negative real part for at least one eigenvalue).*

Simulation configuration for BIOMD003 Goldbeter1991 - Min Mit Oscil

Simulation Type

- ☒ Deterministic
- ☐ Stochastic

Plot Settings

Run Simulation

Dynamic Simulation

Dynamic Settings

Dynamic Plot Views

View 1 × New View

Dependent variables

- ☒ C
- ☒ M
- ☐ X

Parameter Scan

Steady State Simulation

Steady State Settings

Parameter Scan

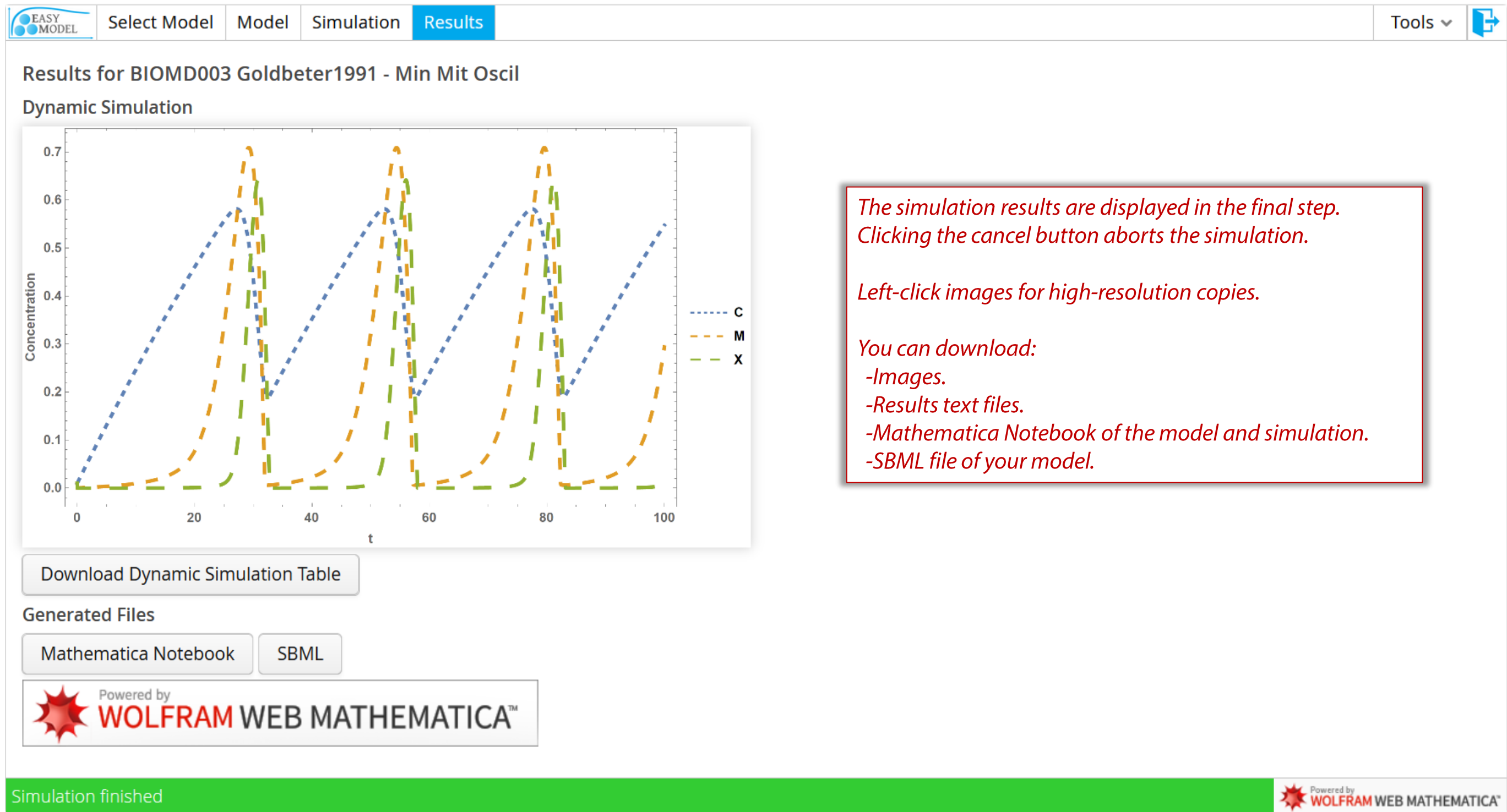
Select Parameters

Select Independent Variables

Reset Selection

Plot views: you can select which time-dependent species are to be plotted in the simulation graphics. Furthermore, you can define several plot views, each of them with its own selected time-dependent species.

Parameter scan: perform the simulation for several values of the rate parameters or independent variables. Select a numerical range and the number of range intervals for the parameter you want to scan to observe how the system evolves with the values variation. Each parameter scan is simulated separated from the others.



You have completed the tutorial!

Press next to start using EasyModel.