Handouts for Object Oriented Modelling in Modelica using OpenModelica

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Part 1: OpenModelica quick start guide

Installation

You can download the OpenModelica software from https://www.openmodelica.org/. We recommend that you download and install version 1.9.6. (accessible at https://build.openmodelica.org/omc/builds/windows/releases/1.9/6/OpenModelica-v1.9.6.exe). After the installation is performed you can run the software in the following way (Windows): search for \bin\OMEdit.exe in Windows Explorer or OpenModelica Connection Editor within the start menu.

Creating and opening a model, loading a library

New objects/models can be created with a new Modelica class by blicking a menu item "File→New Modelica Class" or by using a keyboard shortcut "Ctrl+N". In the window that follows just enter an arbitrary name, e.g. "model_name", to your object. You should save your model afterwards in the file "model_name.mo". Extension ".mo" describes a Modelica object.

You can open existing models by blicking a menu item "File→Open Model/Library File(s)" or by using a keyboard shortcut "Ctrl+O".

Libraries can be used to incorporate several Modelica objects into a single package. This means you can open several objects with a single action. You can load the library into OpenModelica by blicking a menu item "File→Load Library" and selecting the folder that includes your library files together with the "package.mo" file describing the library.

You can now try to load the SysBio library into OpenModelica:

1) Download the SysBio library from http://lrss.fri.uni-lj.si/bio/sysbio/files/SysBio.zip.
2) Unzip the library files.
3) Load the library:
    a. "File→Load Library".
    b. Select the folder in which you unzipped the library files and click "Select Folder".

Afterwards, you can try to load the SteatoNet model, which uses SysBio library (if the library is not loaded before the model, the simulations will not work):

1) Download SteatoNet from http://lrss.fri.uni-lj.si/bio/sysbio/files/SteatoNet.zip.

2) Unzip the file.
3) Open the model:
    a. "File→ Open Model/Library File(s)".
    b. Select the file " NAFLD_model_flux_sensitivity.mo".

Different "Perspectives" and "Views" in OpenModelica

Active perspective can be changed in the bottom right corner of the window (see Figure 1).

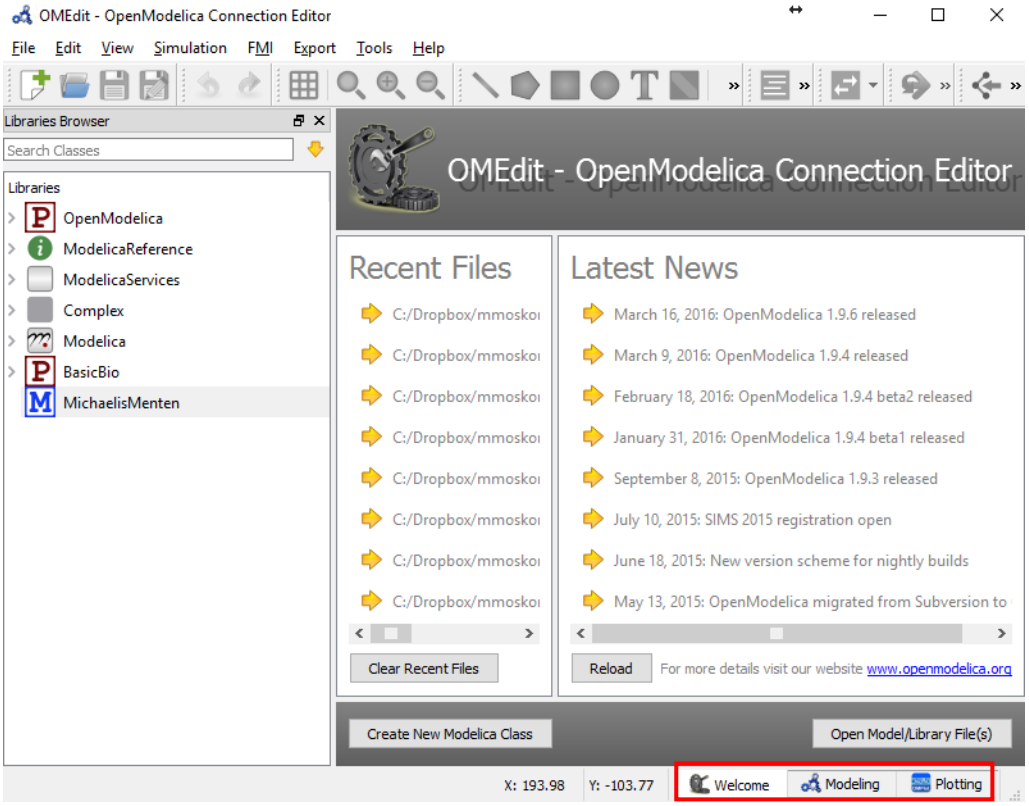

FIGURE 1: OPENMODELICA GREETS YOU IN A "WELCOME PERSPECTIVE". ACTIVE PERSPECTIVE CAN BE CHANGED IN THE BOTTOM RIGHT CORNER OF THE WINDOW.

There are three perspectives possible: "Welcome", "Modeling" and "Plotting".

OpenModelica greets you in the "Welcome" perspective (see Figure 1). Model building can be performed within the "Modeling" perspective. Simulations are performed in the "Plotting" perspective.

"Modeling" perspective

Once you load and open the model (double click on the model file within the "Libraries Browser" menu) perspective is automatically switched to "Modeling" perspective, which allows you to build, modify and browse through your model. "Modeling" perspective has three different views: "Icon View", "Diagram View" and "Text View" (see Figure 2).

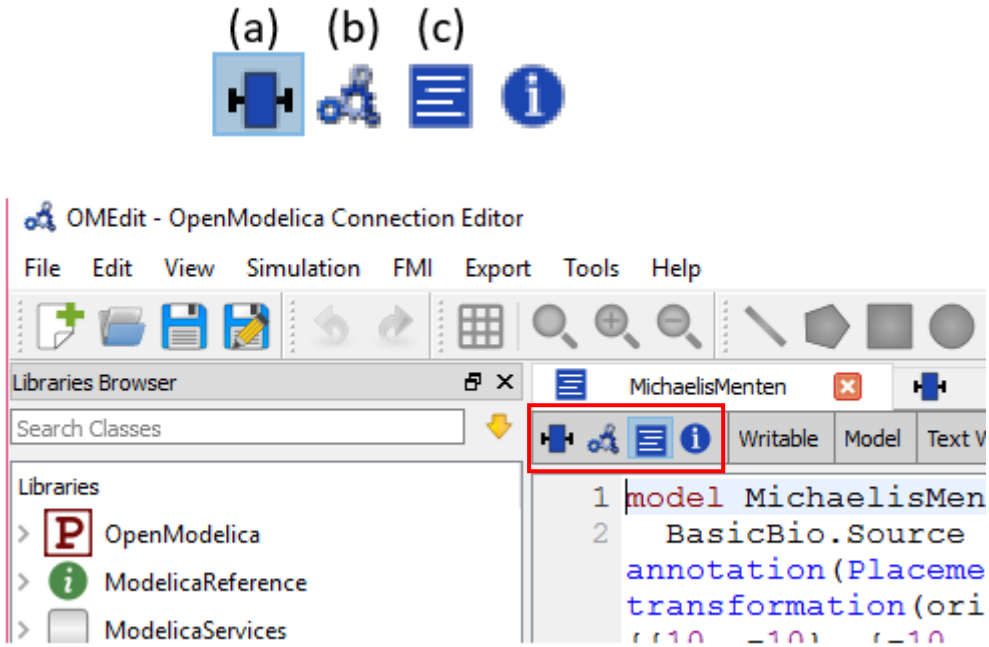

FIGURE 2: DIFFERENT "VIEWS" WITHIN THE "MODELING" PERSPECTIVE. ICON (A) CORRESPONDS TO "ICON VIEW", ICON (B) TO "DIAGRAM VIEW" AND ICON (C) TO "TEXT VIEW".

"Icon View" allows you to design a graphical representation of your model/object. This can be used when building hierarchical models, i.e. models that include other models or objects. Figure 3 represents an "Icon View" for object "Source".

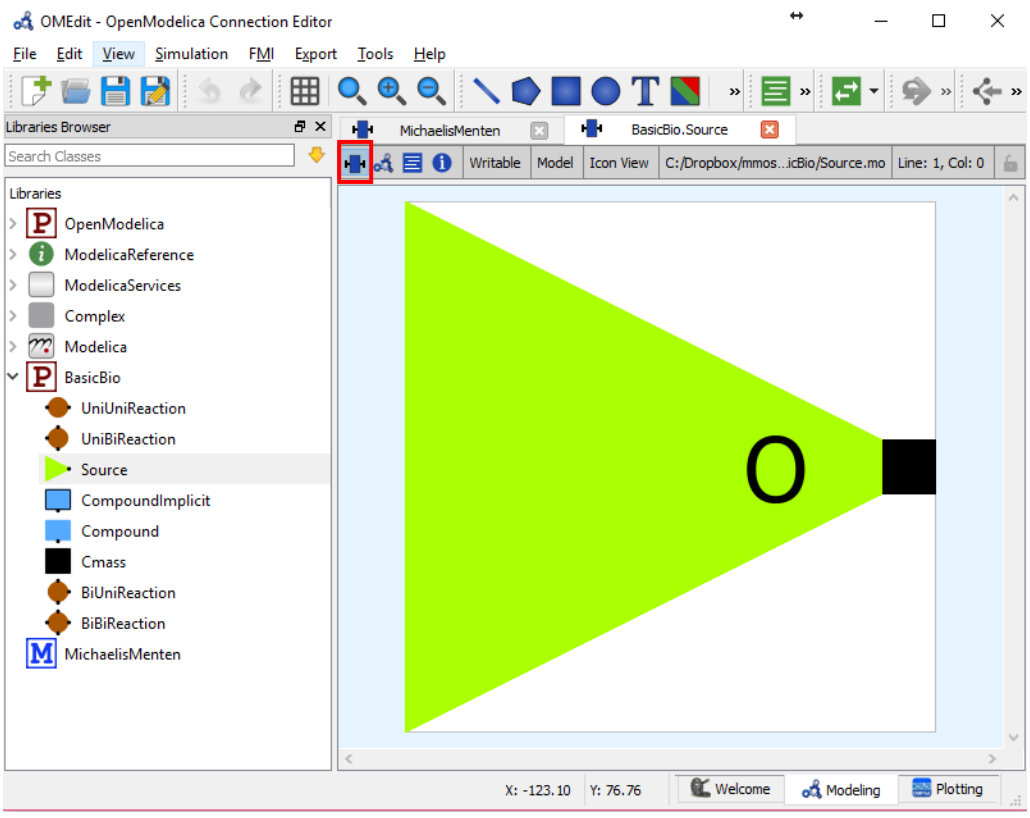

FIGURE 3: ICON VIEW FOR AN OBJECT "SOURCE".

"Diagram view" allows you to build models in a drag-and-drop manner using existing models or objects from the "Libraries Browser". These need to be loaded into OpenModelica before their usage. Figure 4 represents a "Diagram view" of a simple model.

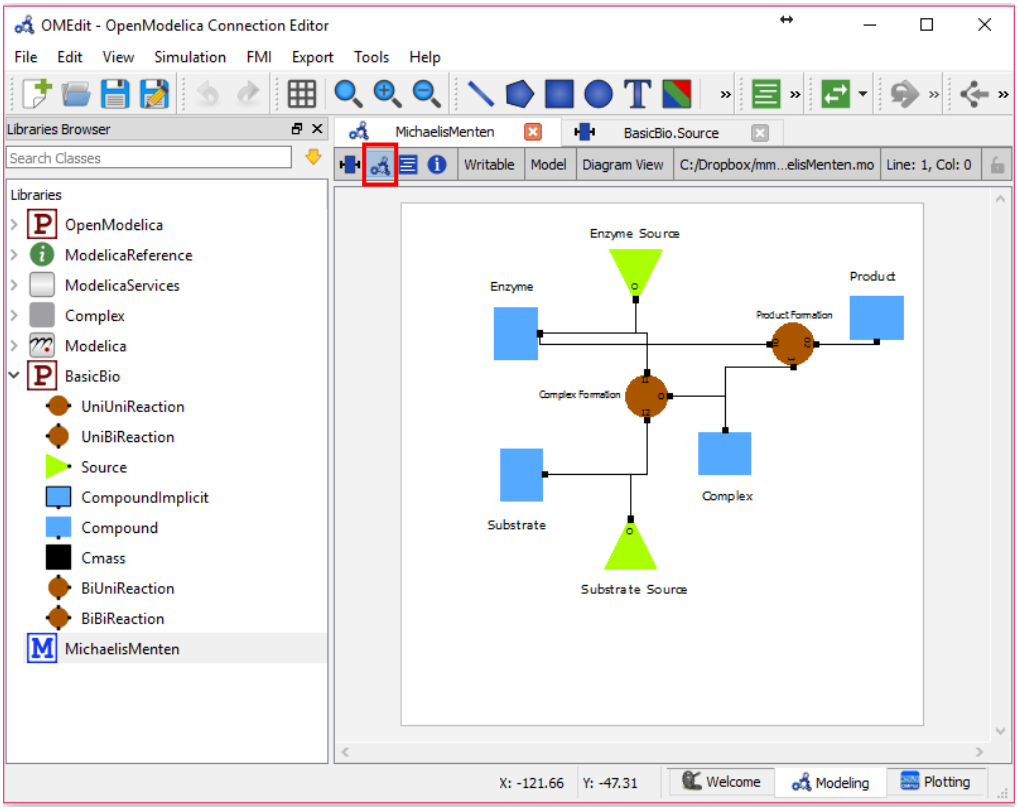

FIGURE 4: "DIAGRAM VIEW" FOR A MODEL "MICHAELISMENTEN".

"Text view" allows you to build models and objects using Modelica programming language (writing the code). Figure 5 represents a "Text view" for the model that was represented graphically in Figure 4.

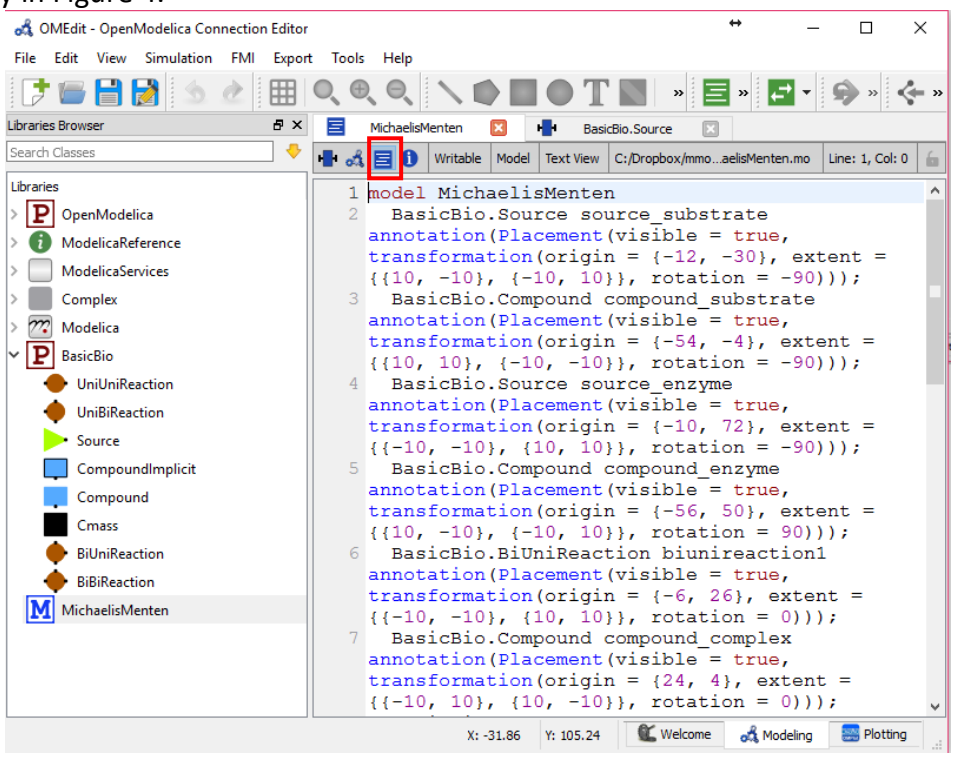

FIGURE 5: "TEXT VIEW" FOR A MODEL "MICHAELISMENTEN".

"Plotting" perspective

Once you initiate the simulations the perspective is automatically changed to "Plotting" perspective, where you can observe the time course of selected variables (see Figure 6). Variables that you want to observe must be selected from the "Variables Browser" menu (right side of the window).

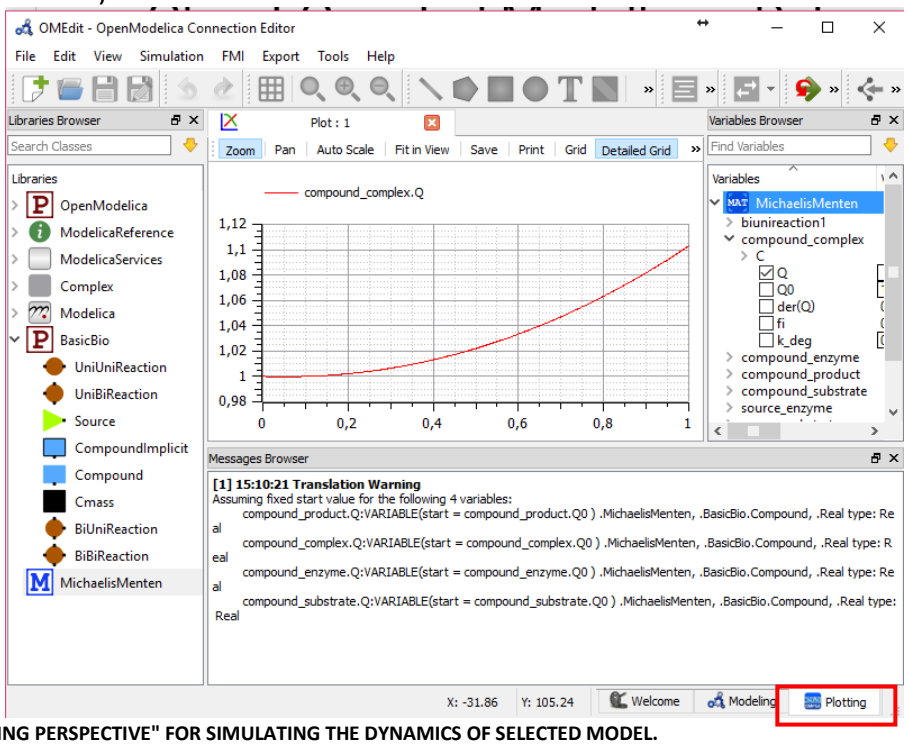

FIGURE 6: "PLOTING PERSPECTIVE" FOR SIMULATING THE DYNAMICS OF SELECTED MODEL.

Building your models

Models can be constructed graphically by using existing models and objects from the "Libraries Browser" menu within the "Diagram View". This option is recommended when you are building relatively small models (i.e. less than 100 objects) and/or when you are only using the basic functionalities of OpenModelica. However, when your models grow in size, it is recommended to use a graphical construction in a combination with textual description, i.e. writing the Modelica code within the "Text View" of the model.

Setting the parameter values

Parameter values that are different than default values can be set in three different ways, i.e. from "Diagram view", "Text view" or "Plotting perspective".

You can access the object properties when using "Diagram view" with a right click on selected object. Parameter values can be set from the "Parameters" window, which is opened after the click (see Figure 7).

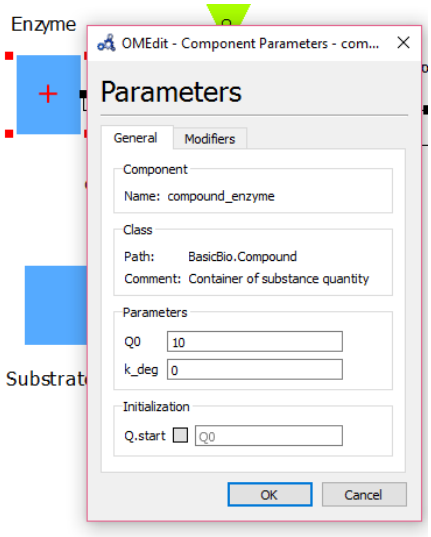

FIGURE 7: SETTING THE PARAMETER VALUES FROM THE "DIAGRAM VIEW".

The modifications you make are also reflected on the code behind your model. You can modify the code directly from the "Text view", giving the parameter values immediately after the object/model declaration, e.g. setting the parameters "Q0" and "k_deg" for the object "compound_enzyme" can be performed with the following code:

```
BasicBio.Compound compound_enzyme(Q0 = 10, k_deg = 0)
```

The third option is to set the parameter values from the simulator's ("Plotting" perspective) "Variable Browser", where you search for an object you want to modify and enter its appropriate parameter values (see Figure 8). It is more convenient to use this option, when you are dealing with large models, because you don't need to recompile the whole model, for the changes to take effect. When you save the model the parameter values are, however, not saved together with the model.

Default parameter values are overridden by the parameter values set within the "Modelling view" (using either "Diagram view" or "Text view"), which are overridden by the parameter values set within the "Plotting" perspective.

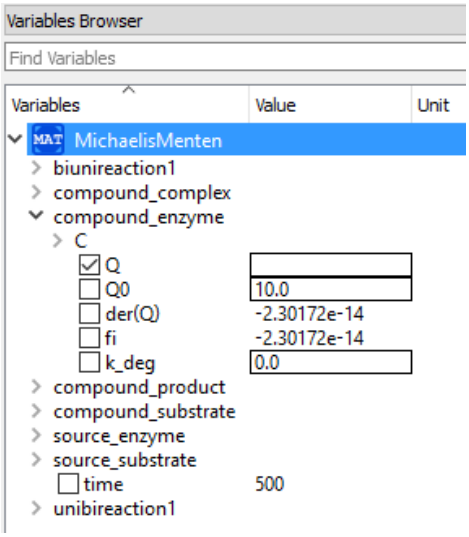

FIGURE 8: SETTING THE PARAMETER VALUES FROM THE "PLOTTING" PERSPECTIVE.

Running the simulations

Simulations can be initiated clicking the menu item "Simulation→Simulate" or simply by clicking in the OpenModelica toolbar. This causes the compilation of the model and automatically changes the perspective to "Plotting" perspective, where you can analyse the simulation results.

You have to manually select the variables you want to plot from the "Variables Browser". You can use the "Find Variables" form to filter out the objects/variables you are interested in (for larger models). Once you find the object and its variable you want to analyse, simply tick mark the box belonging to a variable to plot its time evolution.

If you modify some parameter values within the "Variables browser" you should clear the simulation results of your current simulation using "Clear plot window" icon: and then rerun the simulations with "Resimulate" icon: . If you want to change the simulation setup, such as simulation interval or solver for numerical integration, you should click on the "Re-simulate setup" icon: .

Part 2: Assignments

Assignment 1

1) Load the BasicBio library from the "BasicBio" folder into OpenModelica.
2) Use its objects to construct the model represented with the Figure 9.

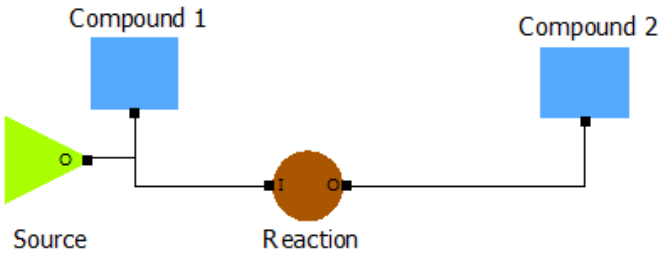

FIGURE 9: GRAPHICAL REPRESENTATION OF ASSIGNMENT 1.

3) Simulate the dynamics of the model using default parameter values.
4) Observe the concentrations of "Compound 1" and "Compound 2".
5) Increase the simulation time to 1000 units.

Solution 1

If you have problems creating your model, you can simply copy-paste the code below into "Text View" of the model:

```
model BasicBio1 BasicBio.Source source1
annotation(Placement(visible = true, transformation(origin =
{-80, 36}, extent = {{-10, -10}, {10, 10}}, rotation = 0)));
BasicBio.Compound compound1 annotation(Placement(visible =
true, transformation(origin = {-60, 56}, extent = {{-10, -10},
{10, 10}}, rotation = 0)));
BasicBio.Compound compound2 annotation(Placement(visible =
true, transformation(origin = {44, 54}, extent = {{-10, -10},
{10, 10}}, rotation = 0)));
BasicBio.UniUniReaction unireaction1
annotation(Placement(visible = true, transformation(origin =
{-20, 30}, extent = {{-10, -10}, {10, 10}}, rotation = 0)));
equation
connect(compound1.C, source1.O) annotation(Line(points = {{-
60, 47}, {-60, 36.5}, {-71, 36.5}, {-71, 36}}));
connect(compound2.C, unireaction1.O) annotation(Line(points =
{{44, 45}, {44, 30}, {-11, 30}}));
connect(unireaction1.I, compound1.C) annotation(Line(points =
{{-29, 30}, {-60, 30}, {-60, 47}}));
annotation(Icon(coordinateSystem(extent = {{-100, -100}, {100,
100}}, preserveAspectRatio = true, initialScale = 0.1, grid =
{2, 2})), Diagram(coordinateSystem(initialScale = 0.1),
graphics = {Text(origin = {-78, 17}, extent = {{-10, 5}, {8, -
3}}, textString = "Source"), Text(origin = {-54, 67}, extent =
{{-20, 9}, {10, -5}}, textString = "Compound 1"), Text(origin
= {-20, 19}, extent = {{-10, 5}, {12, -7}}, textString =
```

```
"Reaction"), Text(origin = {50, 65}, extent = {{-20, 9}, {10,
-5}}, textString = "Compound 2")}));
end BasicBio1;
```

Once you increase the simulation time you should obtain the simulation results as represented in Figure 10.

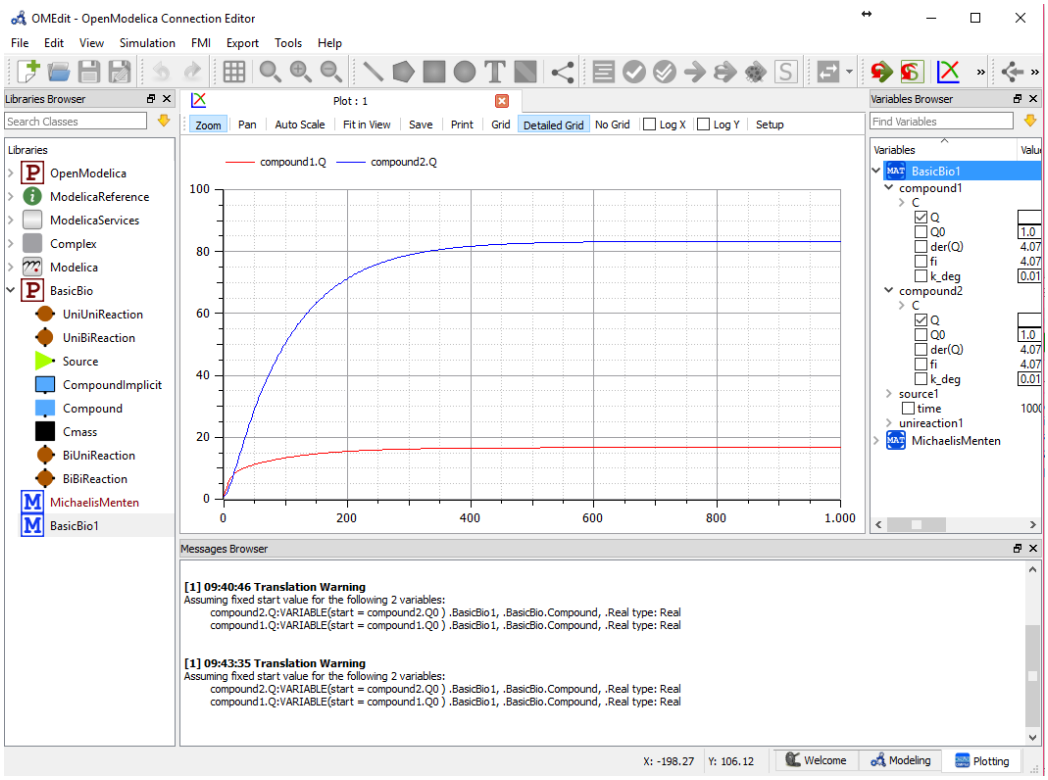

FIGURE 10: SIMULATION RESULTS OF ASSIGNMENT 1 WITH DEFAULT PARAMETER VALUES.

Assignment 2

1) Load the model "MichaelisMenten.mo".
2) Set the parameters and initial conditions to obtain the plot represented in Figure 11.

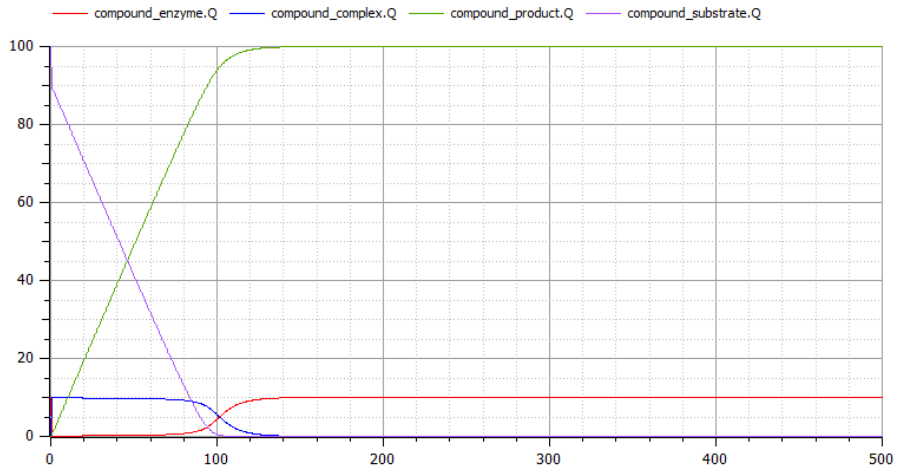

FIGURE 11: MICHAELIS-MENTEN KINETICS.

Solution 2

You can set the parameter values using an arbitrary option described in Part 1 of this document. In order to obtain the required dynamics, you should make the following modifications to default parameter values:

1) Initial substrate concentration ("Q0") should be significantly higher than initial enzyme concentration ("Q0"). Set the initial substrate concentration to 100 and initial enzyme concentration to 10.
2) All input fluxes should be set to 0. Set the output flux of substrate source ("fi") and output flux of enzyme source ("fi") to 0.
3) All degradation rates ("k_deg") should equal 0. Set the substrate degradation rate, enzyme degradation rate, complex degradation rate and product degradation rate to 0.
4) We have to presume that the product formation is an irreversible reaction. Set the reversibility of product formation reaction ("kB") to 0.

Assignment 3

1) Load the SysBio library from "SysBio" folder into OpenModelica.
2) Load the model "CaseStudy\SteatoNet.mo".
3) Simulate the dynamics of the model using default parameter values.
4) Set the perturbation from normal diet to glucose rich diet:
    a. In the "Variables Browser" search for "Glucose_source".
    b. Set the "massflow2" parameter of the object "Glucose_source" to 10.
    c. Set the "switchtime1" parameter of the object "Glucose_source" to 5000.
5) Use the "Re-simulate Setup" window to increase the simulation duration to 60000 units.
6) Display the results:
    a. In the "Variables Browser" search for "SREBP1c_mRNA". Tick mark the variable describing its concentration "Q".
    b. In the "Variables Browser" search for "PPARA_mRNA". Tick mark the variable describing its concentration "Q".

Once you are done you should obtain the simulation results as represented in Figure 12.

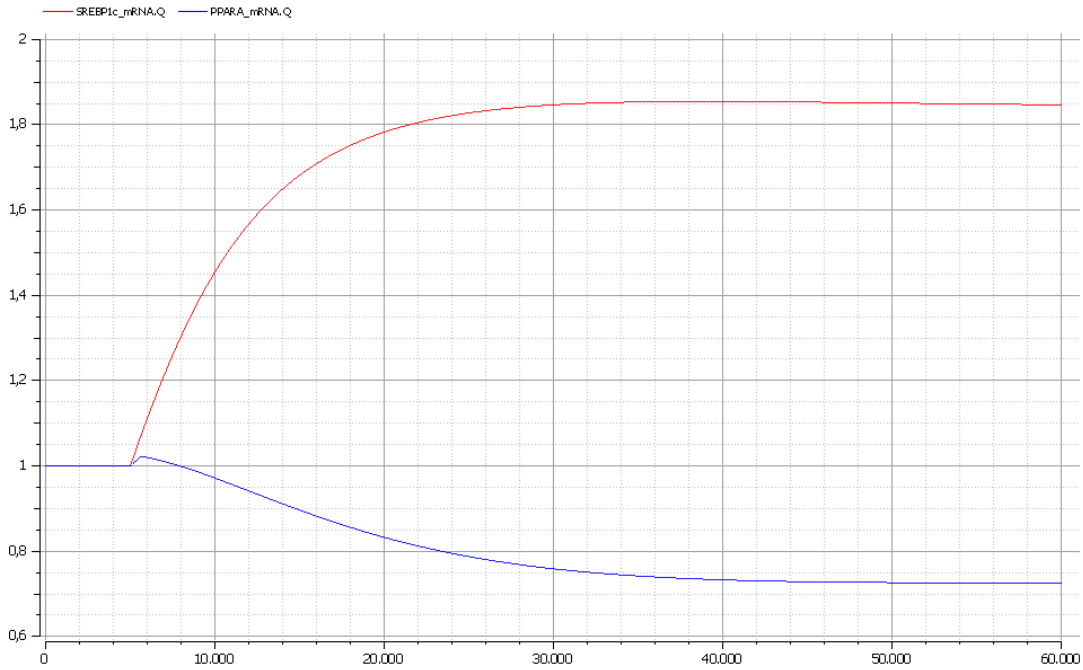

FIGURE 12: SREBP-1C AND PPAR-α TRANSCRIPTOME CONCENTRATIONS BEFORE AND AFTER THE PERTURBATION.