ModTem Tutorial.

1. Introduction

This tutorial describes main features of the Template Application, which is developed to enable the modeller to create a general model-template for a given system and use it for various modelling tasks.
In the tutorial a simple model of the tank mixer is presented and put into Template Application.

2. Preparation of the model

First, what needs to be done, is preparation of the model. The model equations should be derived and composed into three sets of equations – balance, constitutive and connection equations. Also system information should be described, so the model data will be consistent and complete.

3. Example 1 – Steady State Mixer Tank.

In this example, we have mixer tank with 2 streams coming in and one stream going out (Fig. 1). We will perform both mass and energy balance.

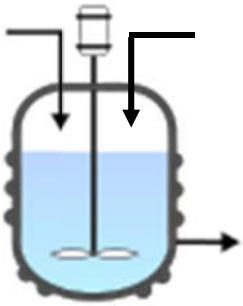

Figure 1. Tank mixer.

Step 1: Describe process system.
There is one system volume, one phase – liquid, and there is no reaction.
Step 2: Define model balances.
There are mass and energy balance equations in our model:
f3[i] = f1[i] + f2[i]
F3*H3 = F1*H1 + F2*H2
Step 3: Define constitutive relations.
In our case these include equations for component enthalpies:
h1[i] =
ADippr103[i]*T1+BDippr103[i]/2*T1^2+CDippr103[i]/3*T1^3+DDippr103[i]/4*T1^4+EDippr103[i]/5*T1^5
h2[i] =
ADippr103[i]*T2+BDippr103[i]/2*T2^2+CDippr103[i]/3*T2^3+DDippr103[i]/4*T2^4+EDippr103[i]/5*T2^5
h3[i] =
ADippr103[i]*T1+BDippr103[i]/2*T1^2+CDippr103[i]/3*T1^3+DDippr103[i]/4*T1^4+EDippr103[i]/5*T1^5
Step 4: Define connection and conditional relations.
This part includes definition of closure equations, which in our case are

F1 = sum_i(f1[i])
F2 = sum_i(f2[i])
F3 = sum_i(f3[i])
H1 = sum_i(h1[i]*f1[i])/F1
H2 = sum_i(h2[i]*f2[i])/F2
H3 = sum_i(h3[i]*f3[i])/F3
T3 = Tmix

Now we are ready to proceed to the template application. Open ICAS and find in the task manager button “ModFrame”(Fig.2). After clicking the button, the interface screen appears (Fig.3). Press the button “ModTem” to run template application.

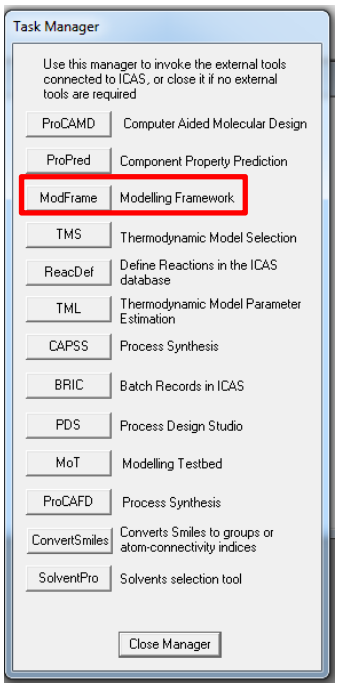

Figure 2. Modelling Framework button in ICAS Task Manager.

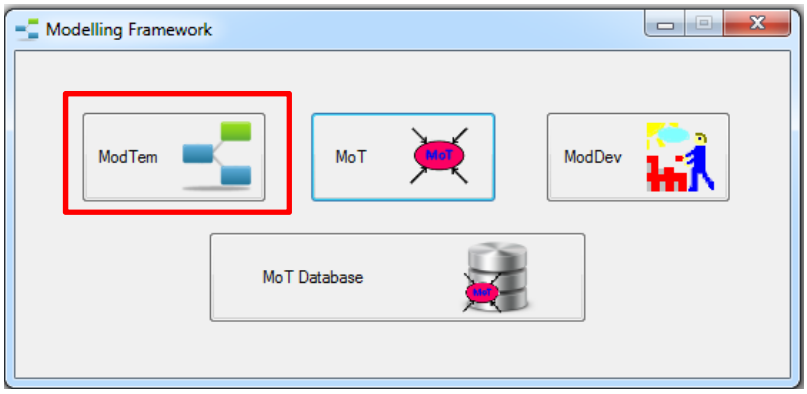

Figure 3. Starting interface.

The starting screen of Template Applications is shown at the Figure 4. As we want to create a new template, click the button “Create new template”.

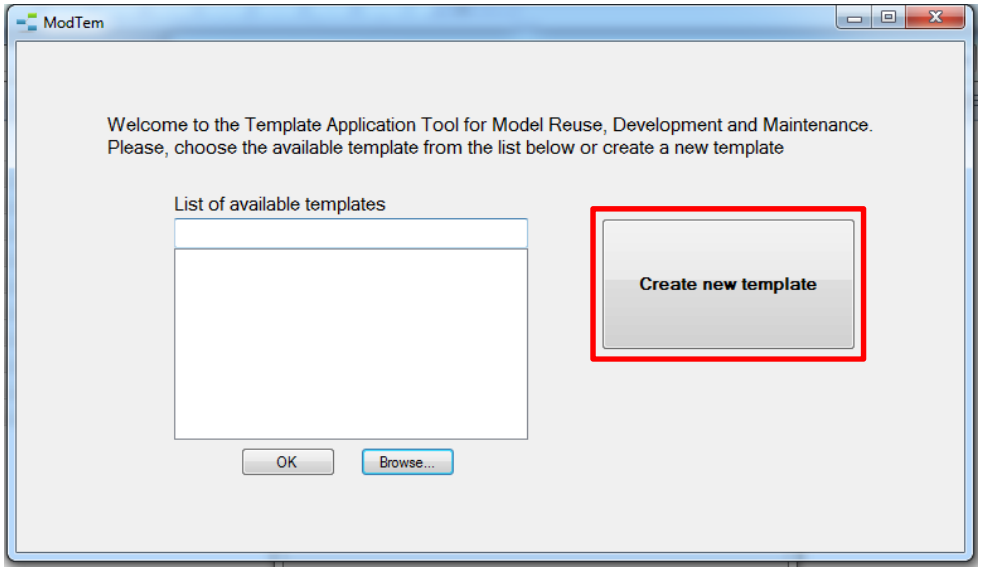

Figure 4. Starting screen of ModTem.

Next window will show the form for a new template creation (Fig. 5). As you can see, there are special layers for each part of the model that we defined before – system information, balance equations, constitutive equations, connection equations.
First, we will give the name for our template, using the top green block. Right click on this block – you will get a field to enter the name (Fig. 6).
Now we will start to describe our system. In the first layer of System Information click the button “Add sub-layer” (Fig. 7). When new sub-layer appears, right click on it to get a field for the name (Fig. 8). This sub-layer is “Number of volumes in the system”.

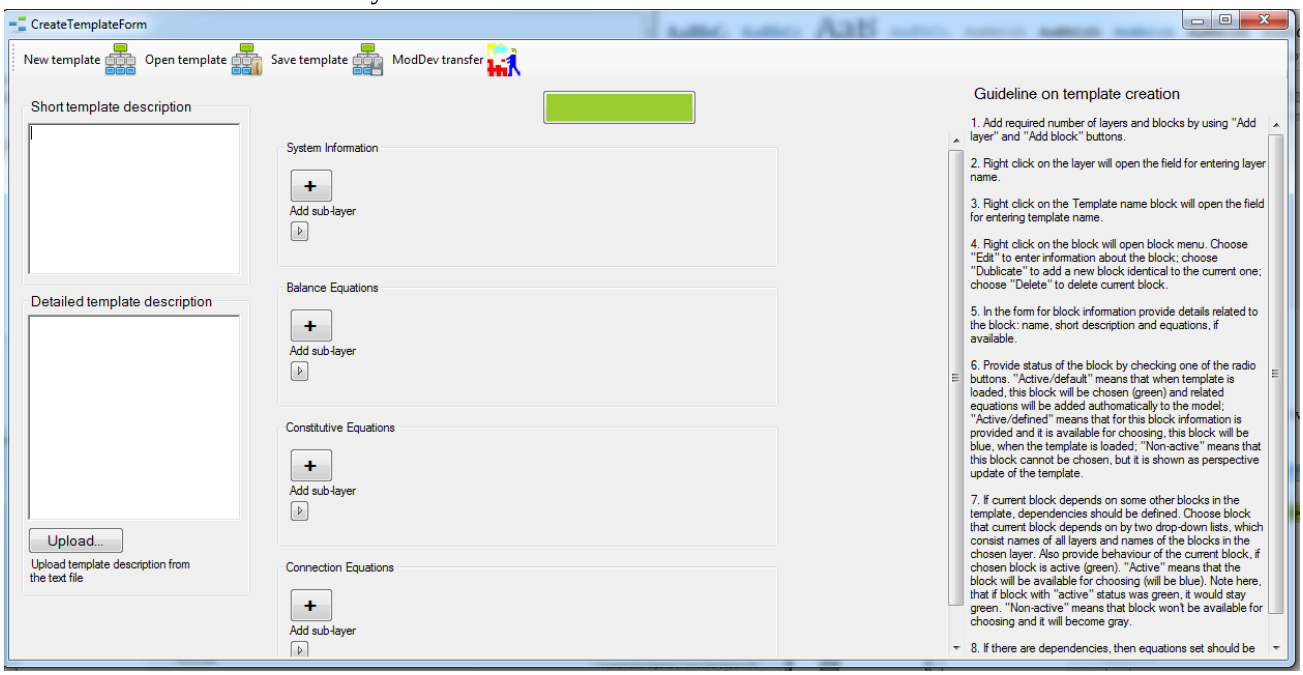

Figure 5. Window for the new template creation.

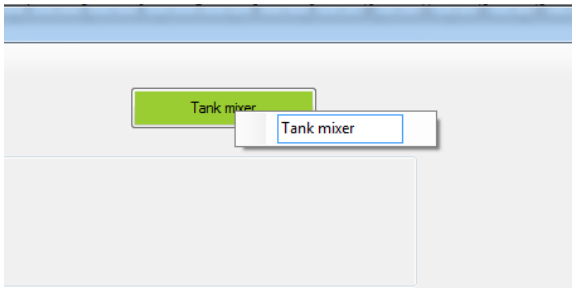

Figure 6. Entering template name.

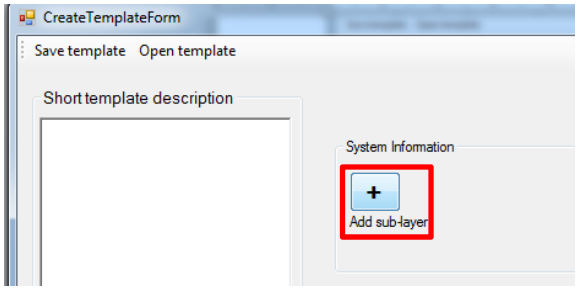

Figure 7. Adding new sub-layer.

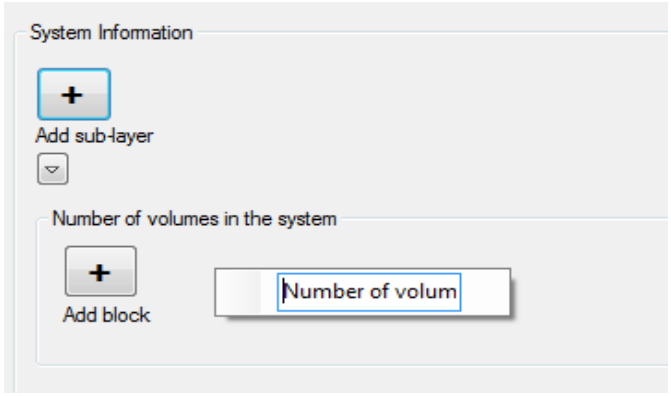

Figure 8. Entering name of sub-layer.

Now, add two more sub-layers in System Information with names “Number of Phases” and “Presence of reaction” (Fig. 9).

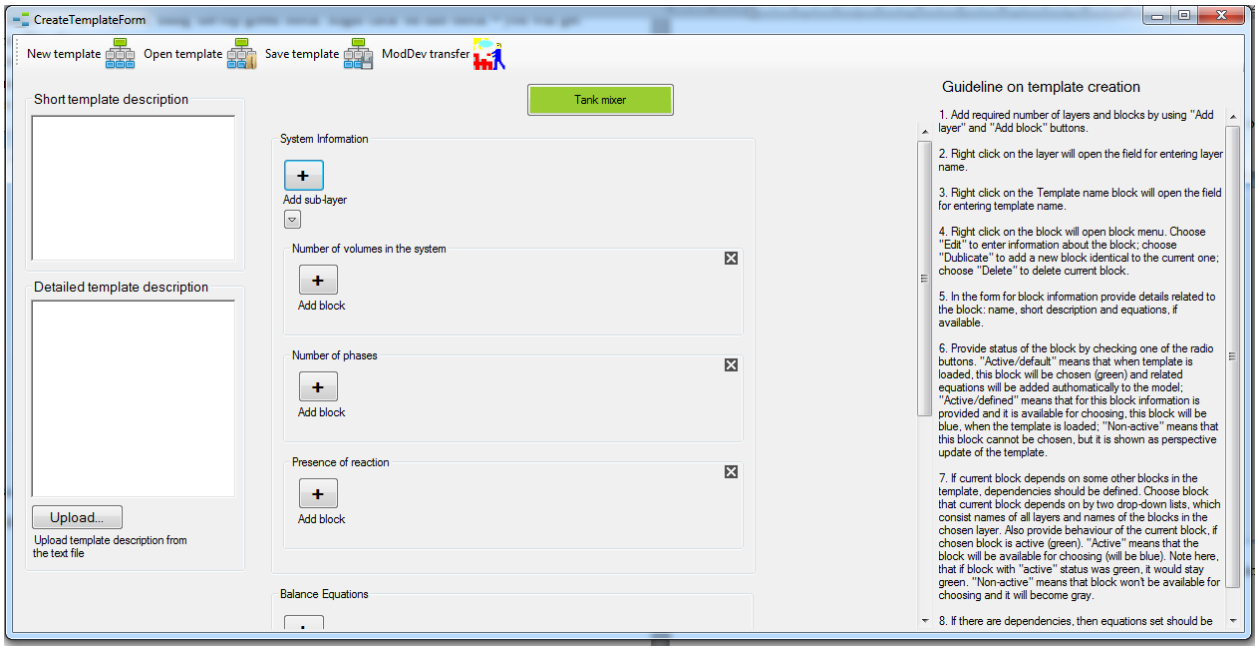

Figure 9. Template application screen after adding sub-layers to System Information.

Next step is to add blocks to the new sub-layers.
Click the button “Add block” in the first sub-layer of System Information (Fig. 10). Now, when the block appears, right click on it and choose “Edit” from the context menu (Fig. 11).

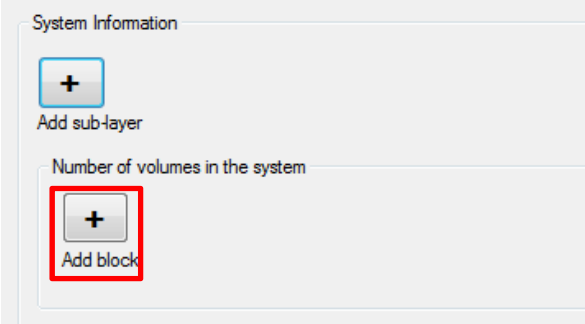

Figure 10. Adding a new block to sub-layer.

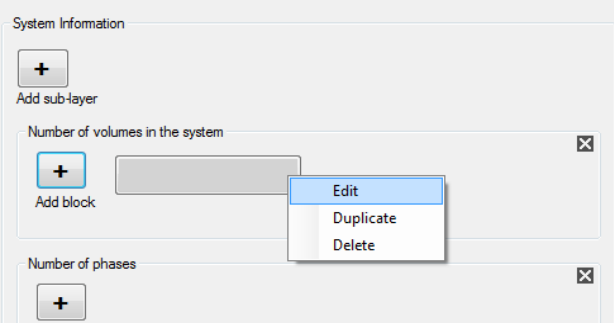

Figure 11. Context menu of the block.

A new form for block information is shown (Fig. 12). Here we should provide all information related to the block. First, we enter name of the block. Since this block is related to the number of volumes in the system and there is only one volume, so we will put the name “One”. Next, provide short description, which gives some details about the role of this block in the template. At last we will define block behaviour; this shows how the block will appear in the template, when it will be used. There are three options: Active/Default – block is chosen by default, it will have green color and its equations will be added to the model, when template is called; Active/Defined – block could be chosen by user, it has blue color and its equations will be added to the model, if user will click it; Non-active – block cannot be chosen by user, it is grey, this option can be used, when there is no information for this block currently, but it might be described later. There are no equations or dependencies for this block, so these parts are left empty (they will be explained later). Figure 13 shows the information form after being filled. Click OK to save changes and to close the form.

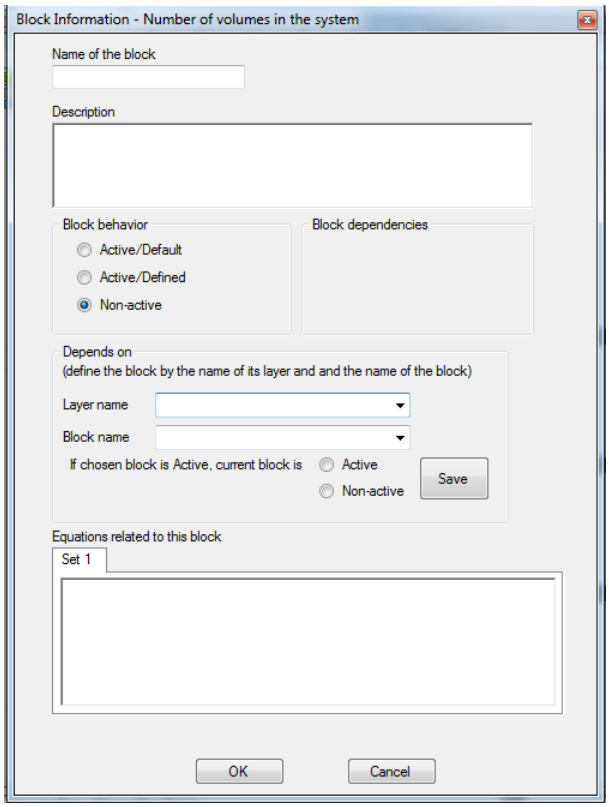

Figure 12. Block information form.

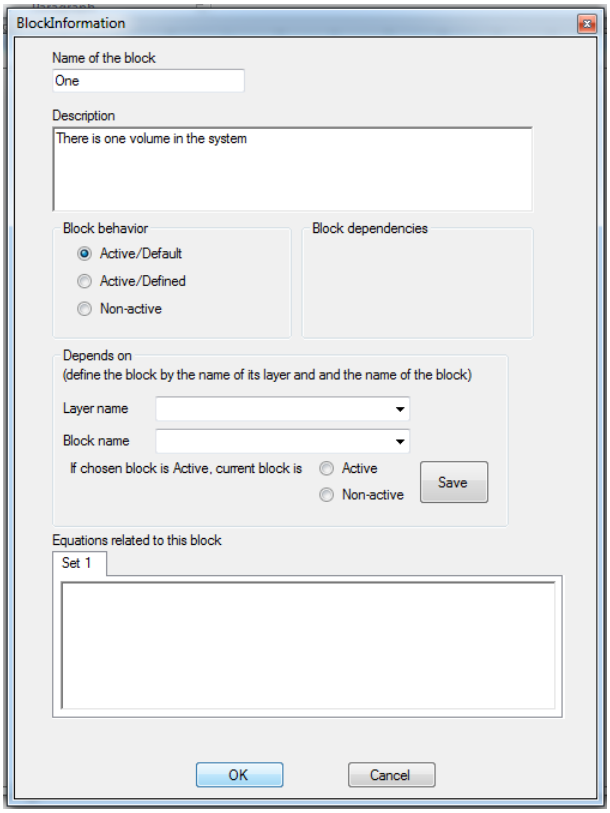

Figure 13. Filled block information form.

Now we can see changes in our template after describing the first block (Fig. 14). Add and fill out two more blocks in the sub-layers “Number of phases” and “Presence of reaction”. See figures 15-18 for details.

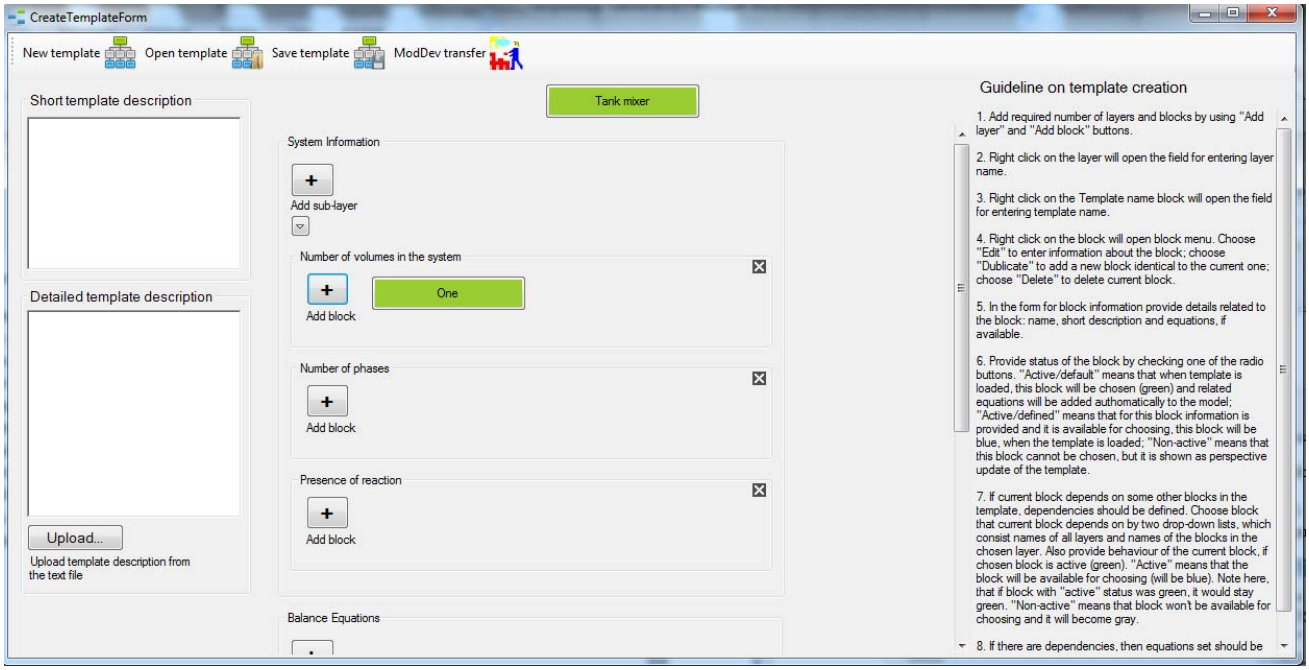

Figure 14. Template creation screen after adding and describing first block.

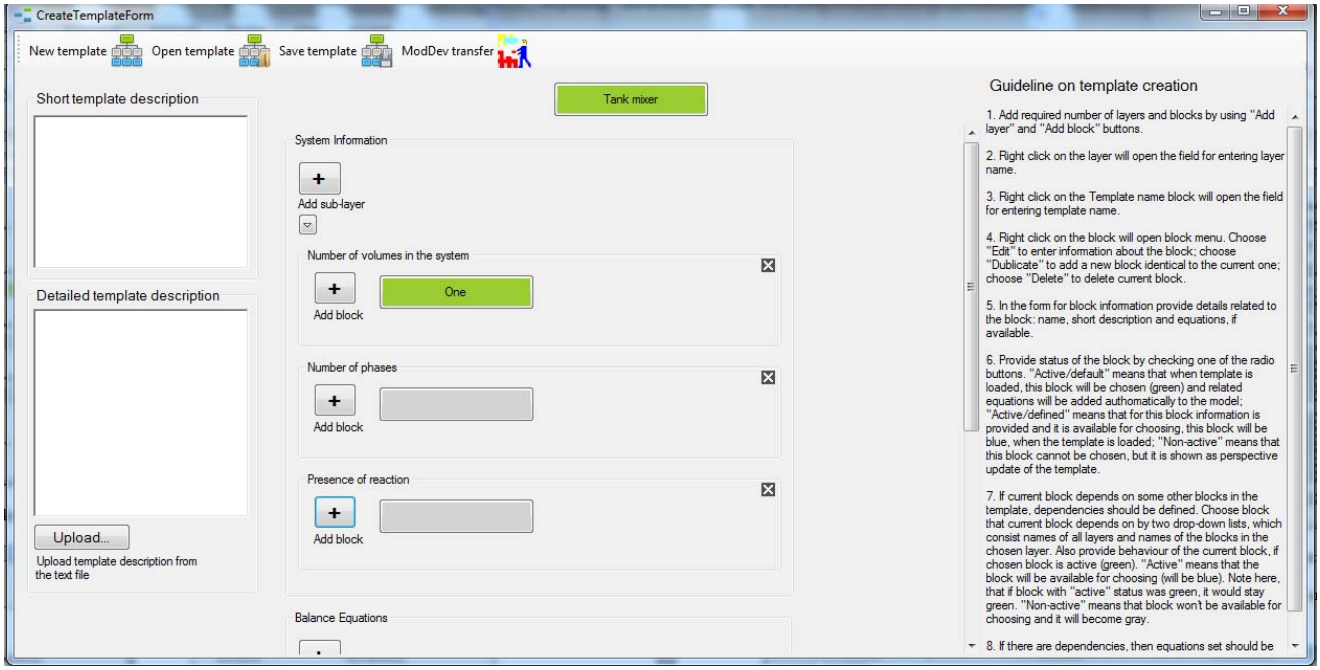

Figure 15. Two more blocks are added to other sub-layers.

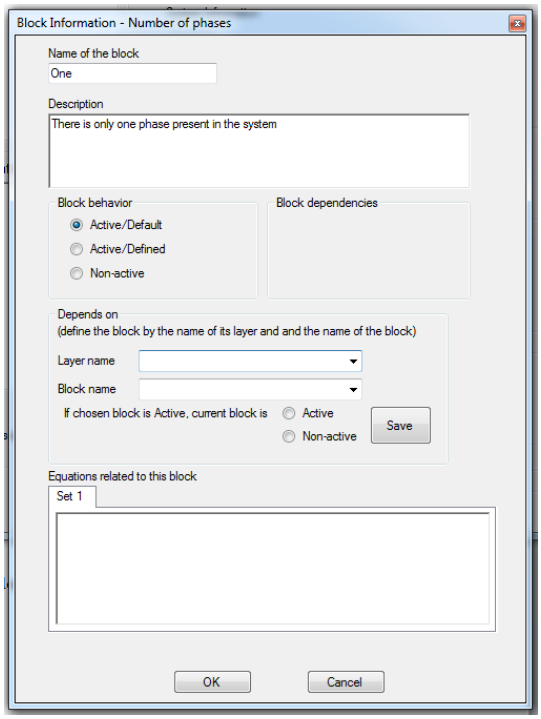

Figure 16. Block information of the second block.

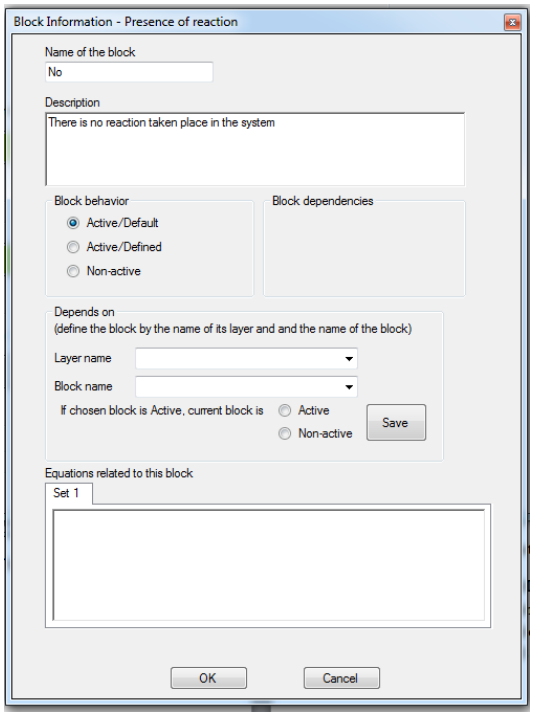

Figure 17. Block information of the third block.

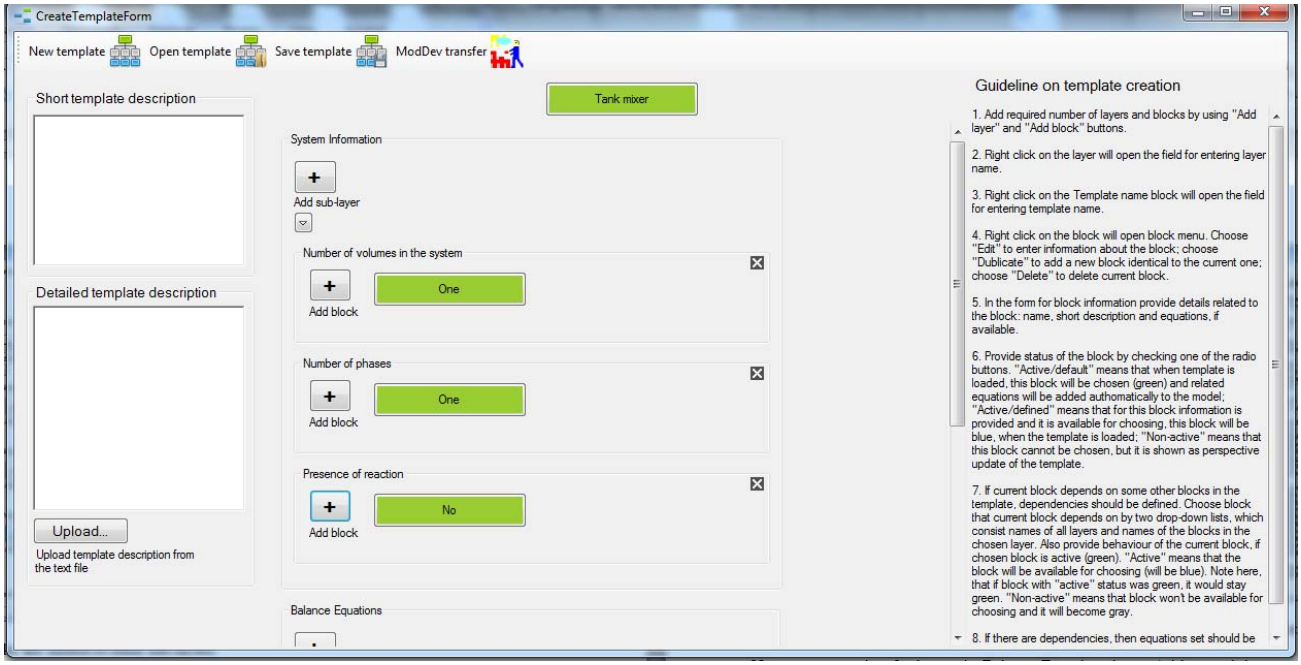

Figure 18. Template creation screen after adding and describing all blocks in System Information layer.

Now we are moving further to the Balance Equations layer. Add two sub-layers and name them “Mass balance” and “Energy balance” (Fig. 19).

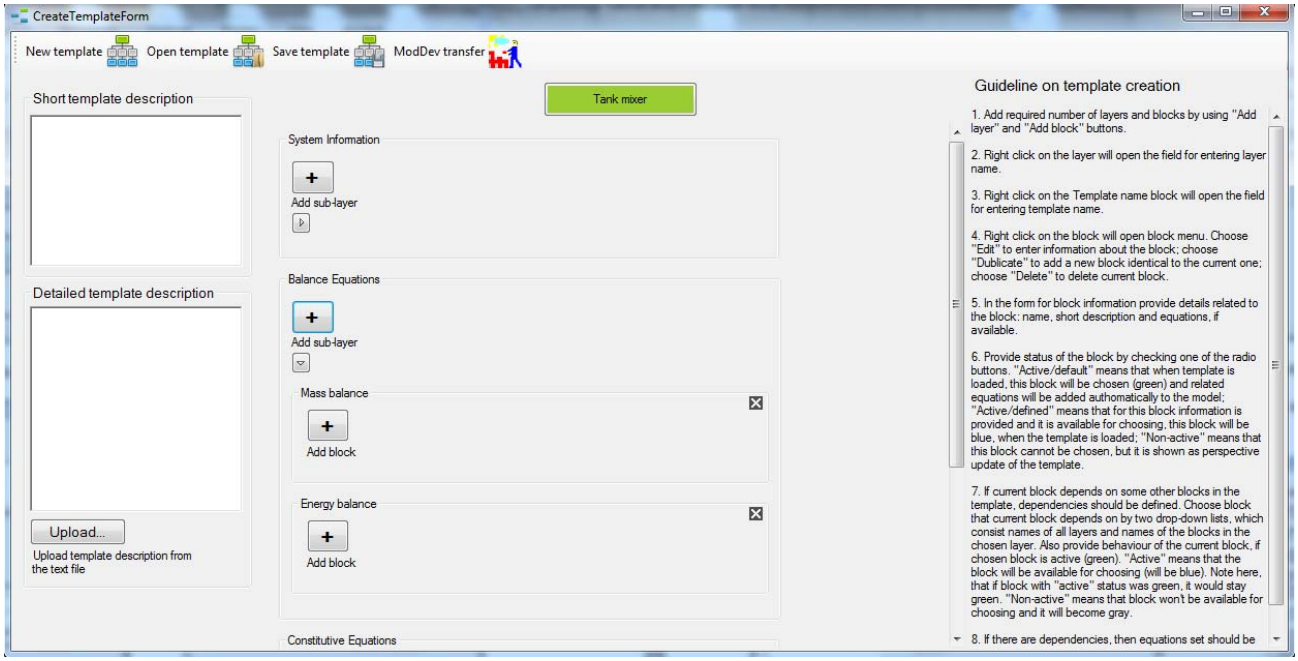

Figure 19. Template creation screen after adding sub-layers for balance relations.

Add new block to the “Mass balance” sub-layer and open the information form. Apart from the name, description and block behaviour, we will provide mass balance equation, which we defined previously. Put this equation in the text window at the bottom of the information form. After providing all information click OK to save result. See figure 20 for details.

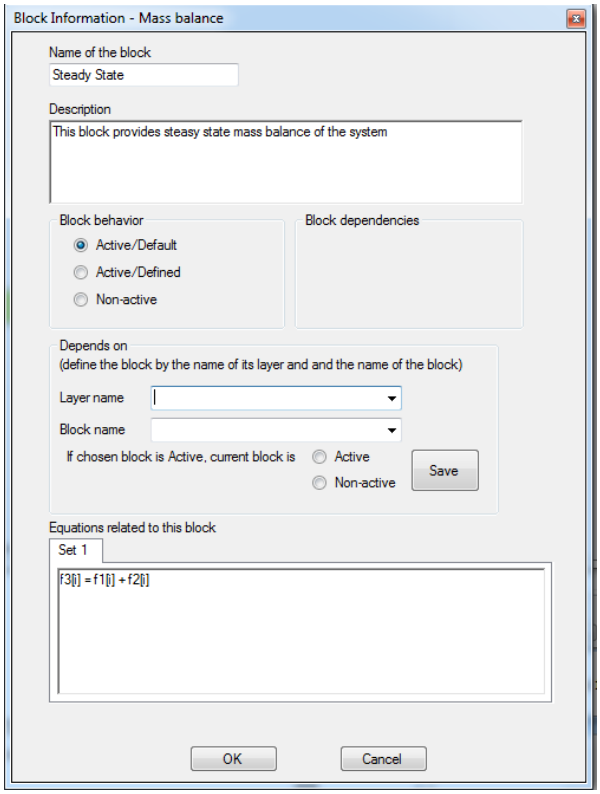

Figure 20. Information form for the block describing mass balance.

Now we will add one more block to “Mass balance” sub-layer. We will define it as “Dynamic State”. Although we don’t have equations for dynamic state mass balance, but it is very likely that we might describe it later. For now this block will have “non-active” status (see fig. 21, 22).

As a next step we will add block to “Energy balance” sub-layer. It will be block, describing steady state energy balance of our system, we can as well provide equations from our model (see fig. 23, 24).

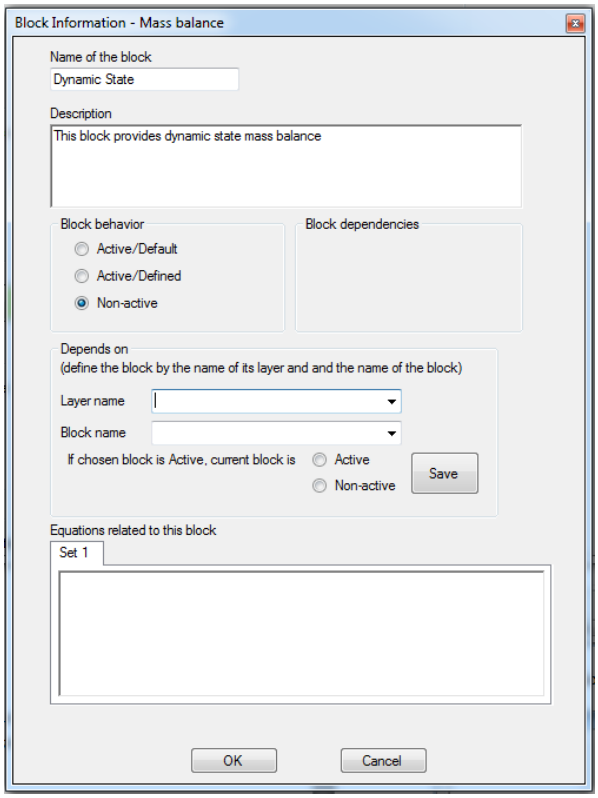

Figure 21. Information form for non-active block.

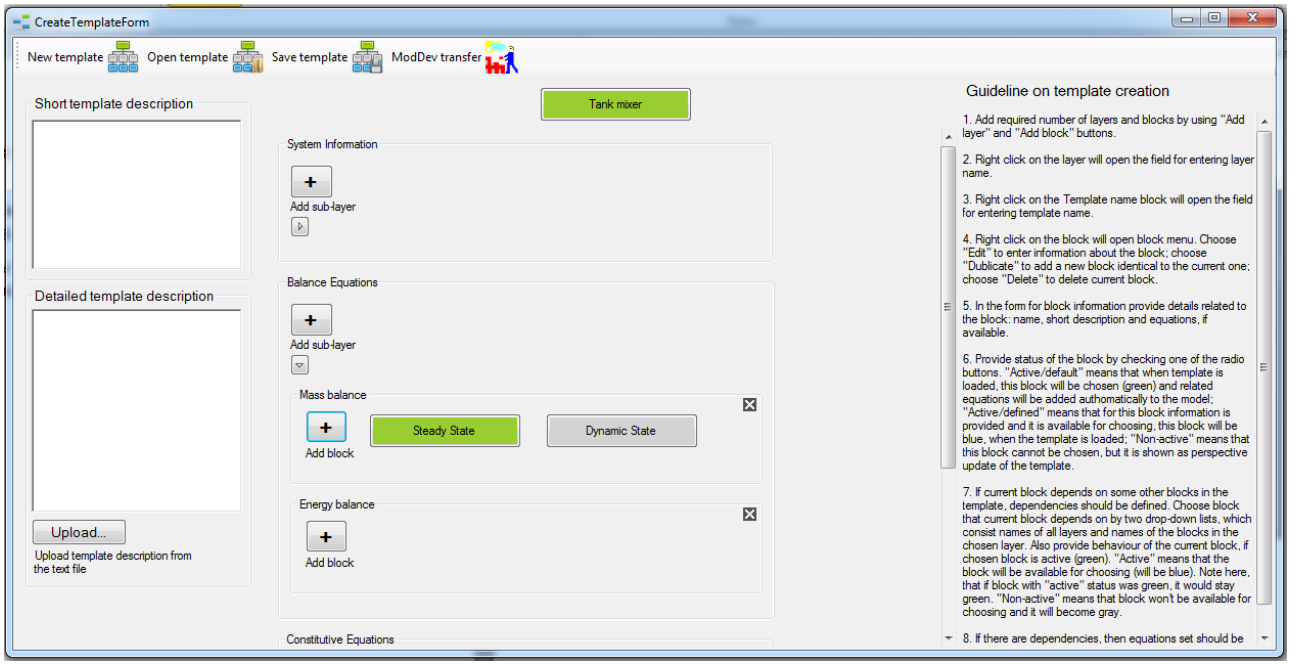

Figure 22. Template creation screen after adding and describing block for “Mass balance” sub-layer.

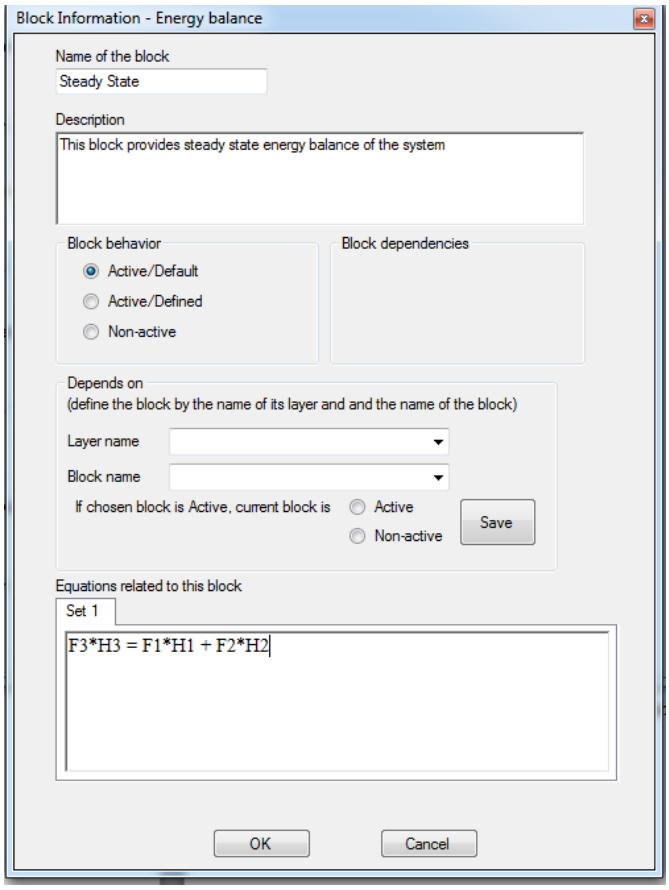

Figure 23. Information form for energy balance block.

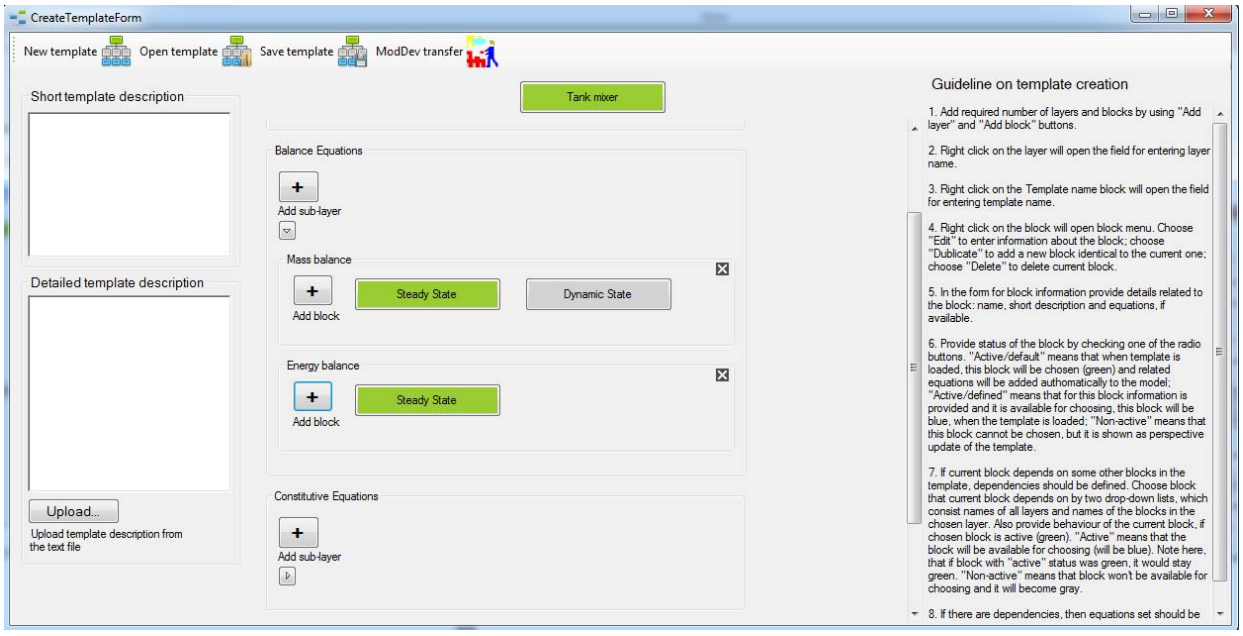

Figure 24. Template creation screen after filling out layer “Balance Equations”.

Now we are moving to “Constitutive equations” layer. Here we are adding one sub-layer named “Enthalpies”, where we also add one block – “Enthalpy correlations”. See Figures 23 and 24 for details.

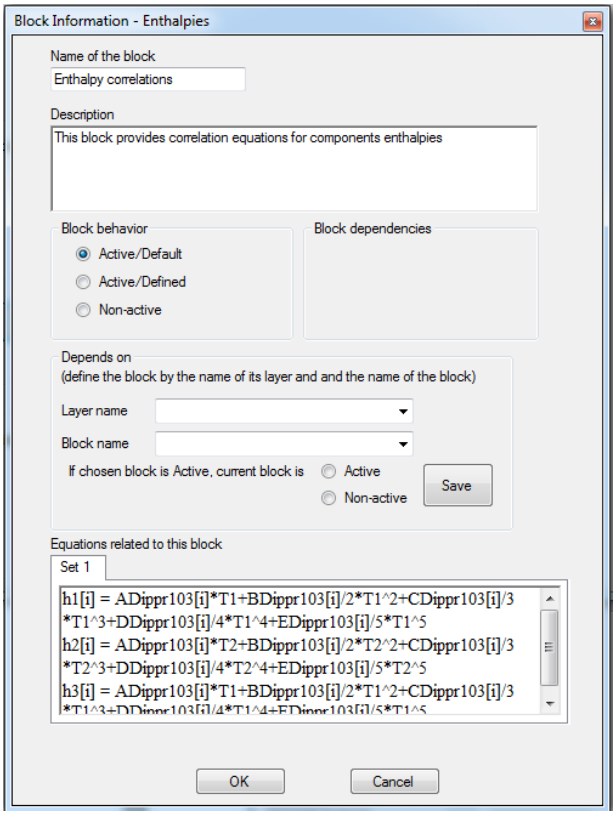

Figure 25. Information form for block related to constitutive equations.

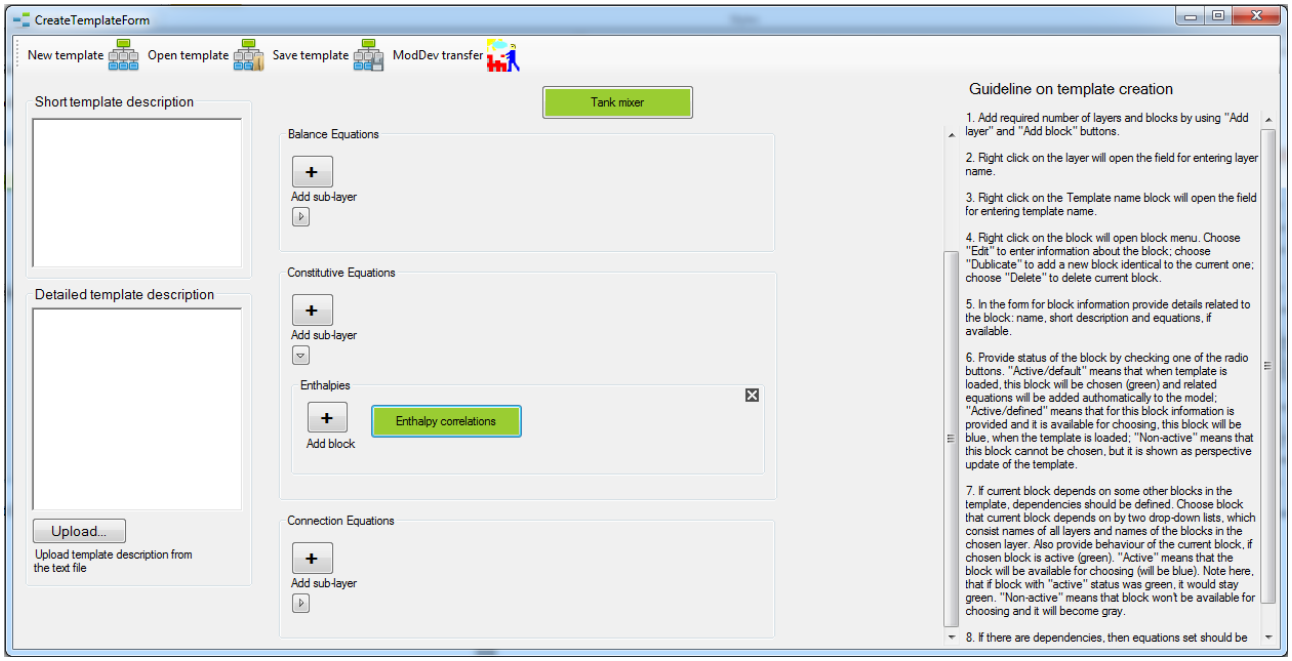

Figure 26. Template creation screen after filling out layer “Constitutive Equations”.

And the last layer we need to fill is “Connection Equations”. In our case we have only closure equations to add. Create new sub-layer and block in it to describe our closure equations (see fig. 27, 28).

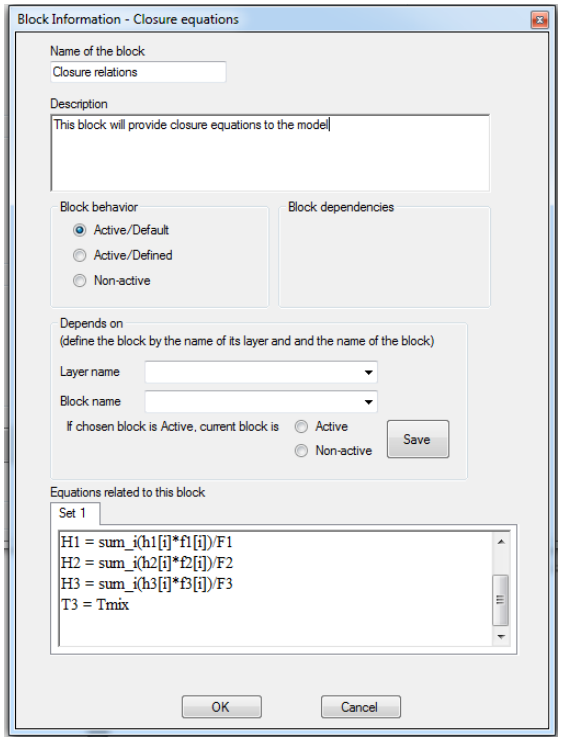

Figure 27. Information form of the block for closure equations.

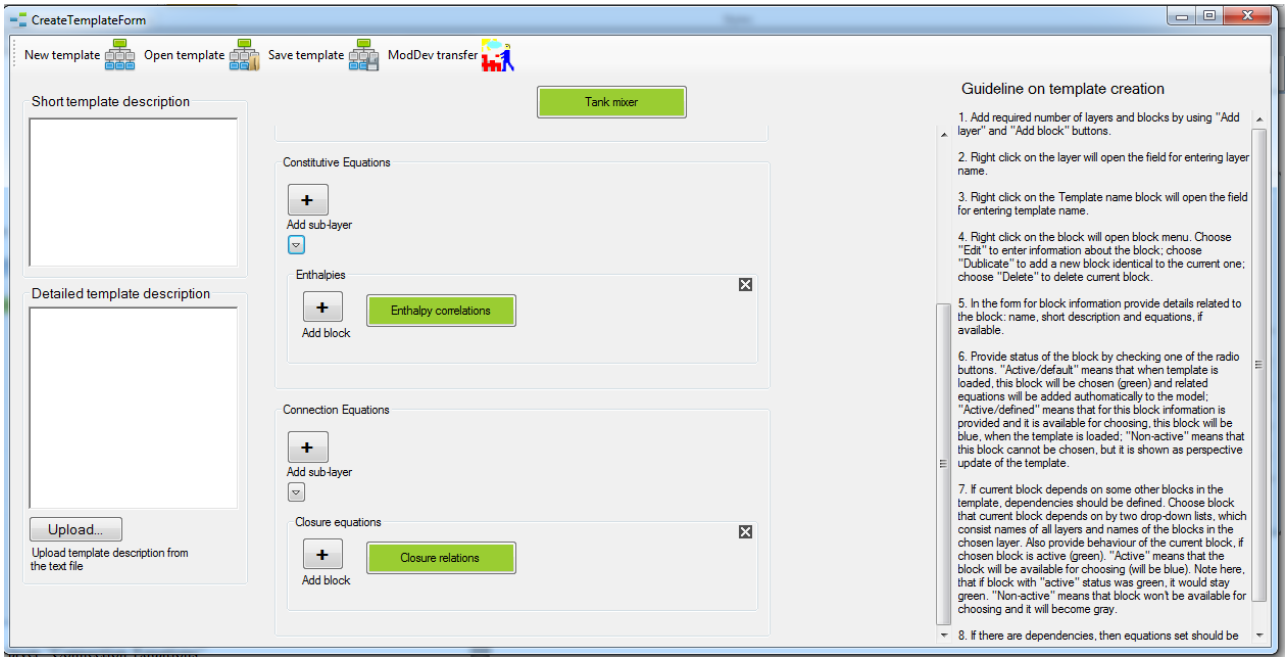

Figure 28. Template creation screen after filling out layer “Connection Equations”.

Now in order to finish our template, provide template description in the test field on the left side of the screen. Click “Save template” (Fig. 29).

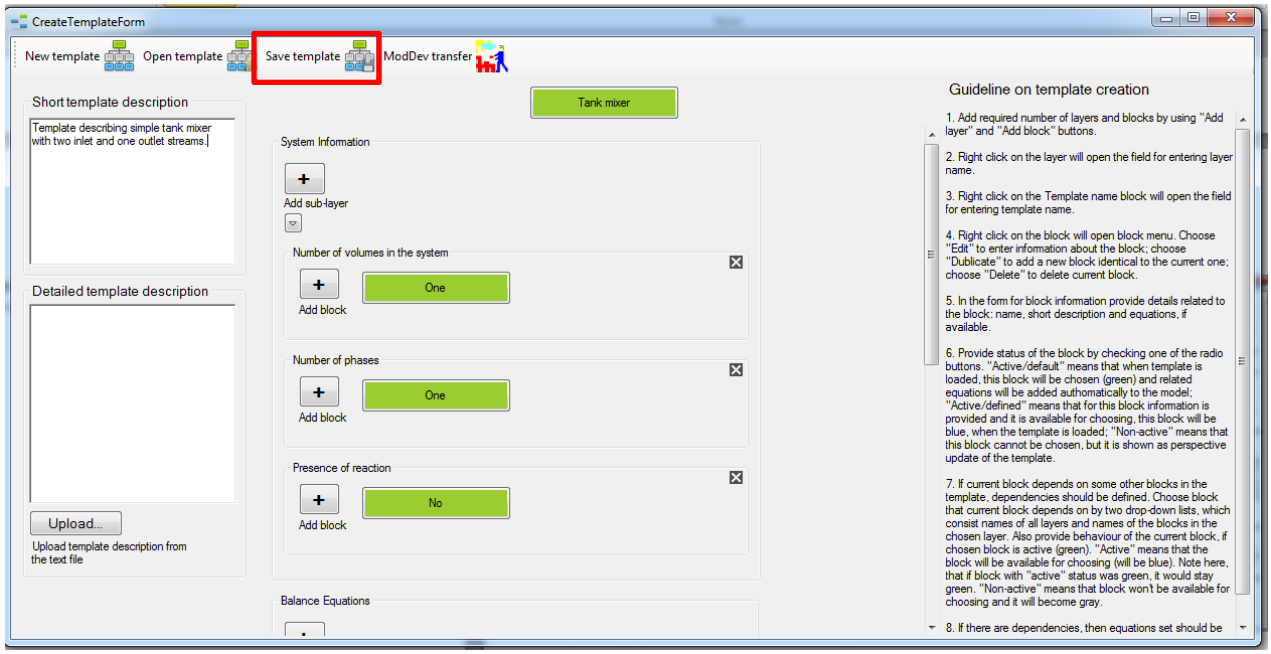

Figure 29. Template creation screen after filling template description.

Provide the name of the file and a folder (Fig. 30). Then our template will be saved.

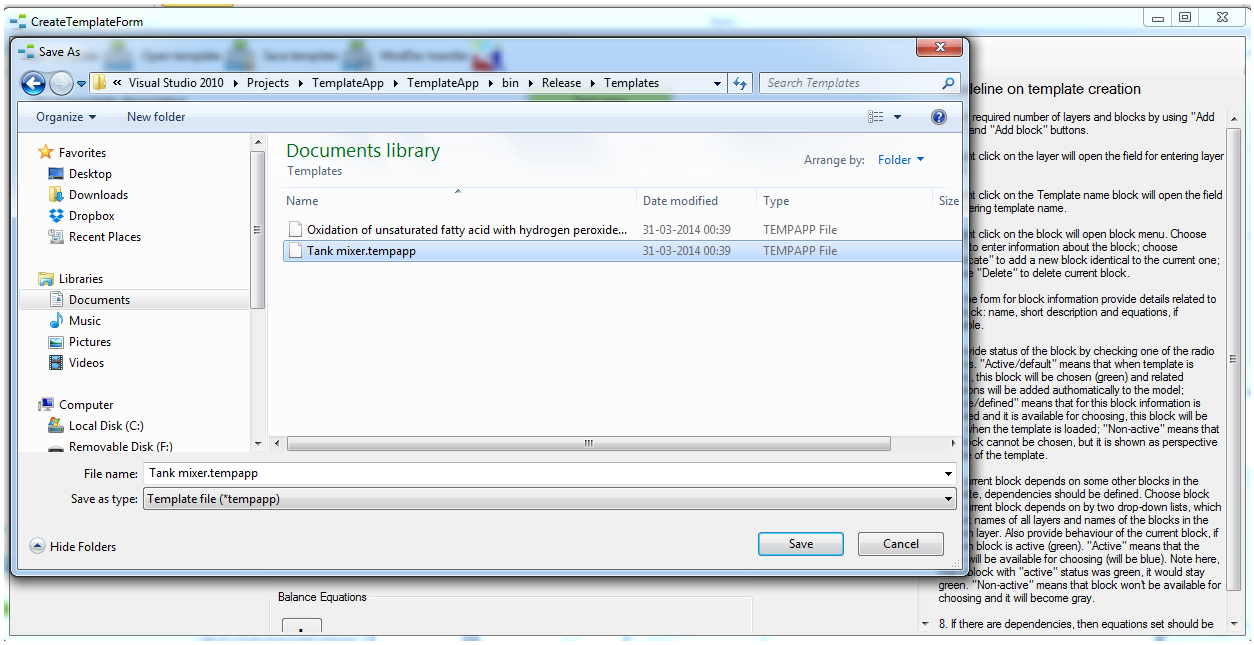

Figure 30. Saving of the template.

4. Example 2 – Open created template.

Now close template creation screen and go to the starting form of Template Application. Click “Browse…” to open file dialog and find the template file of our tank mixer (Fig 31, 32).

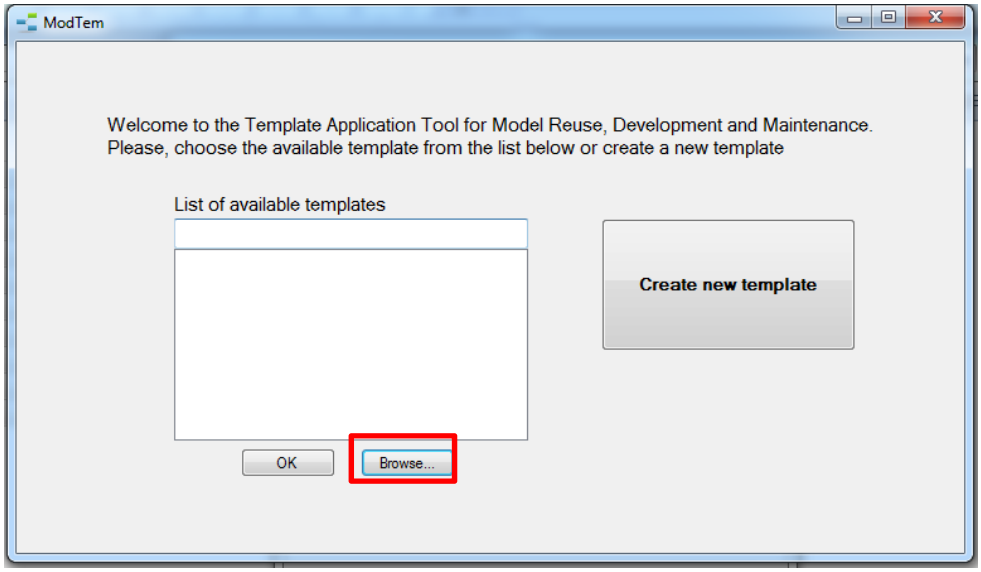

Figure 31. Opening existing template.

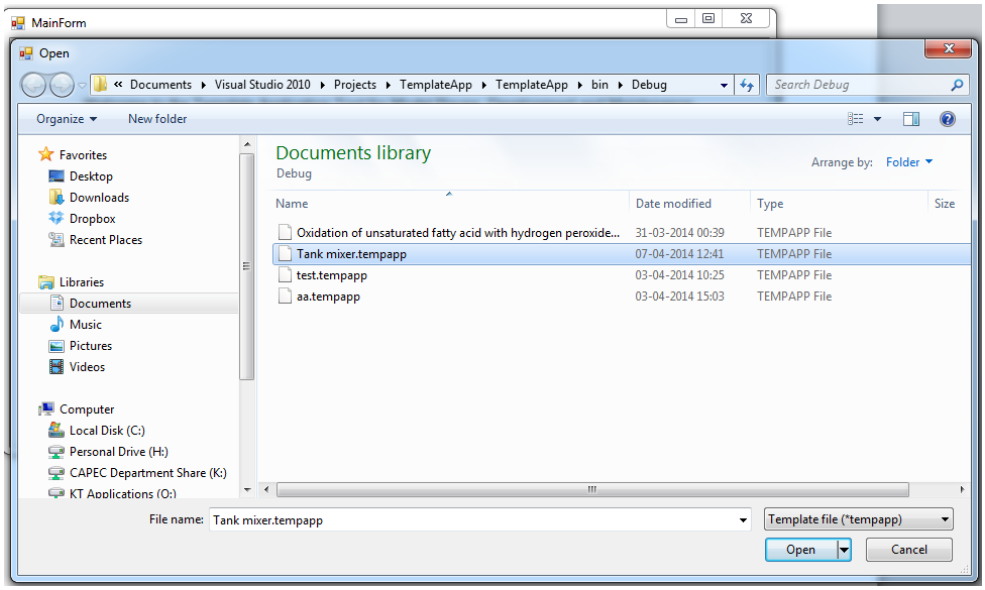

Figure 32. Opening existing template.

The screen with template will be opened. Note, that all equations from default blocks are already added to the text field on the right side (Fig. 33).

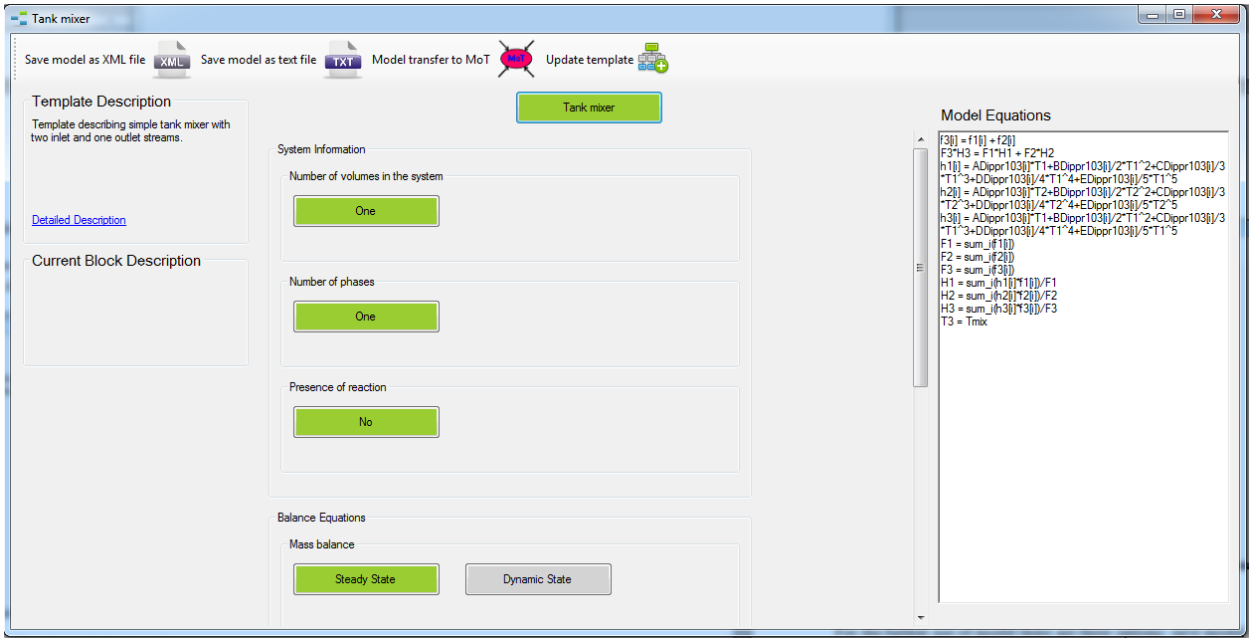

Figure 33. Template use screen with tank mixer template.

For the further use of model there are three options: save model to xml file, txt file or transfer directly to MoT. To save model to the file, click the corresponding button from the tool menu (Fig. 34). Afterwards provide the name of the file and click “Save”, so the model will be saved (Fig. 35).

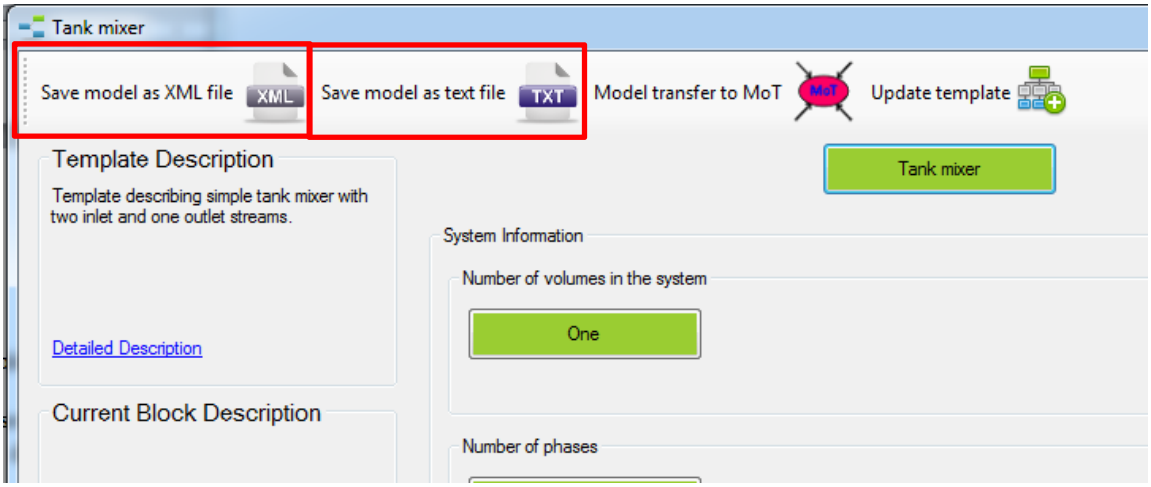

Figure 34. Tool menu of the template screen.

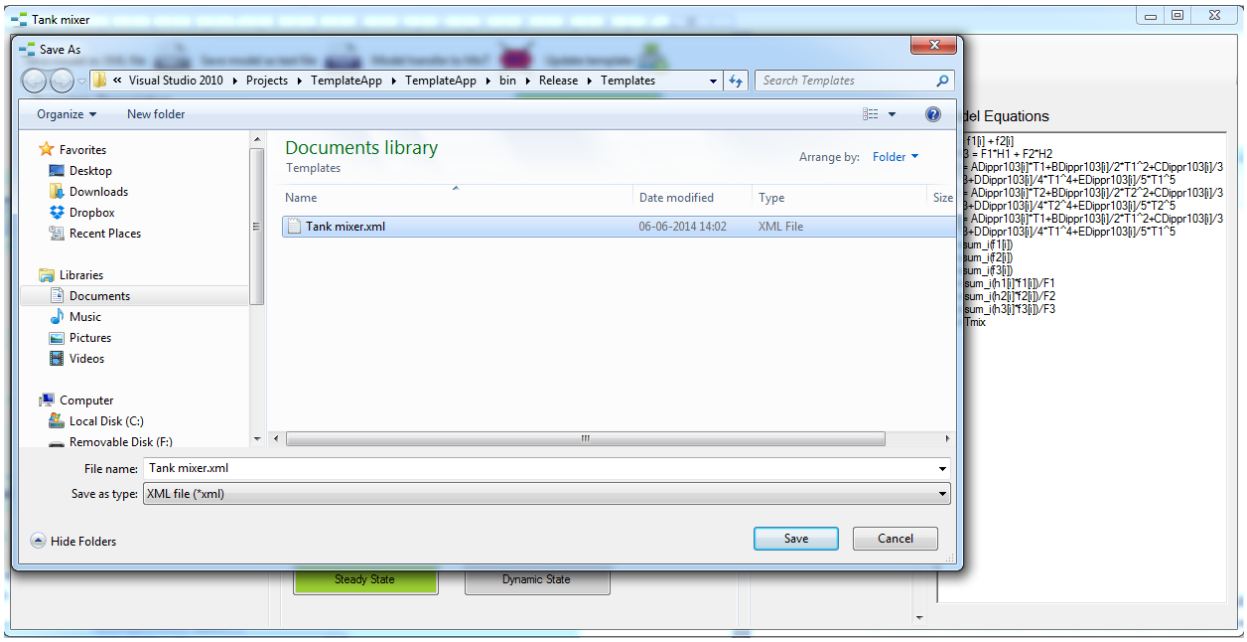

Figure 35. Saving template as xml file.

Another option is to transfer model directly to MoT. After clicking at the button, MoT will be open with already translated model of our tank mixer (Fig 36, 37).

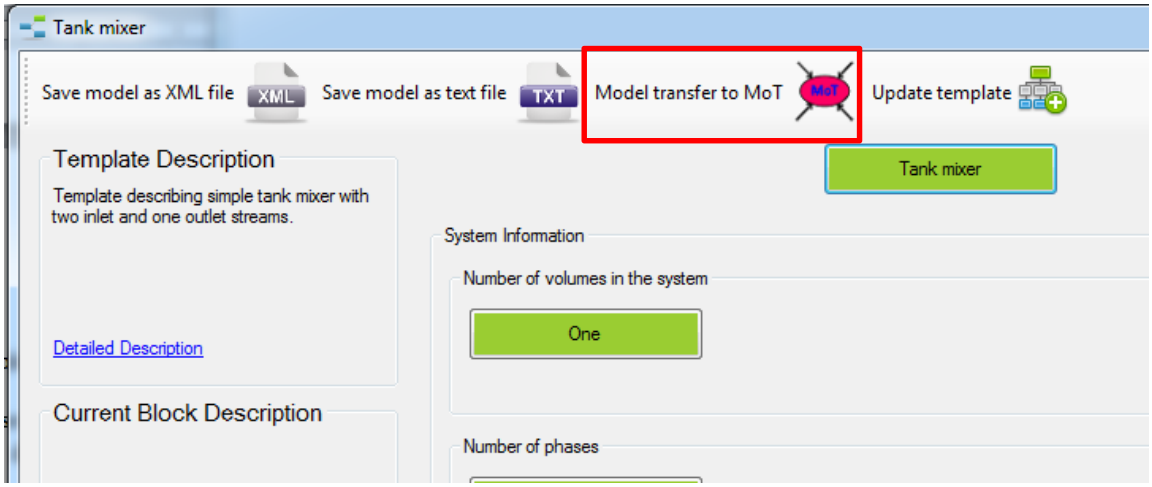

Figure 36. Button to transfer model to MoT.

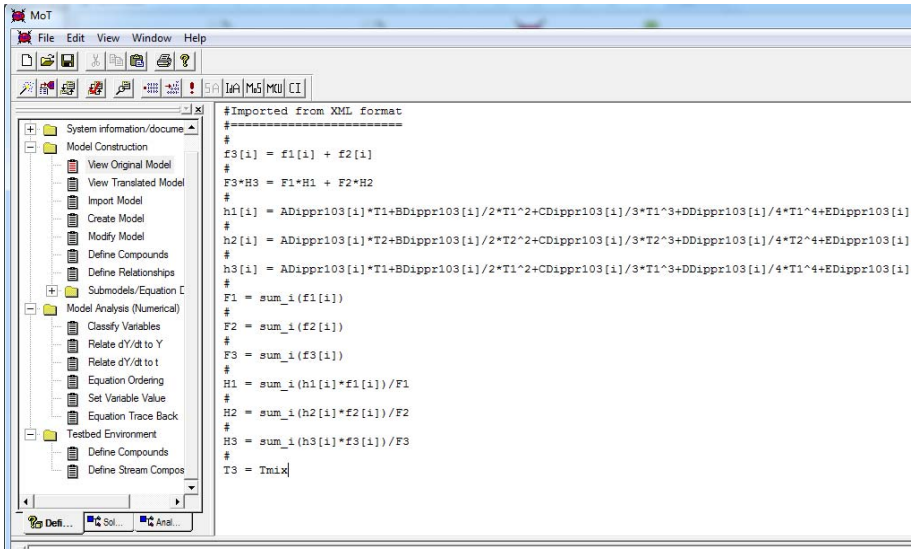

Figure 37. MoT screen with transferred model.

5. Example 3 – Update the template; use of dependencies.

Now we will make updates in our tank mixer template. Originally we had two streams coming into tank, now we will consider the situation, when there are three streams entering tank.

To go again to the template creation screen, click “Update template” button in the tool menu (Fig 38).

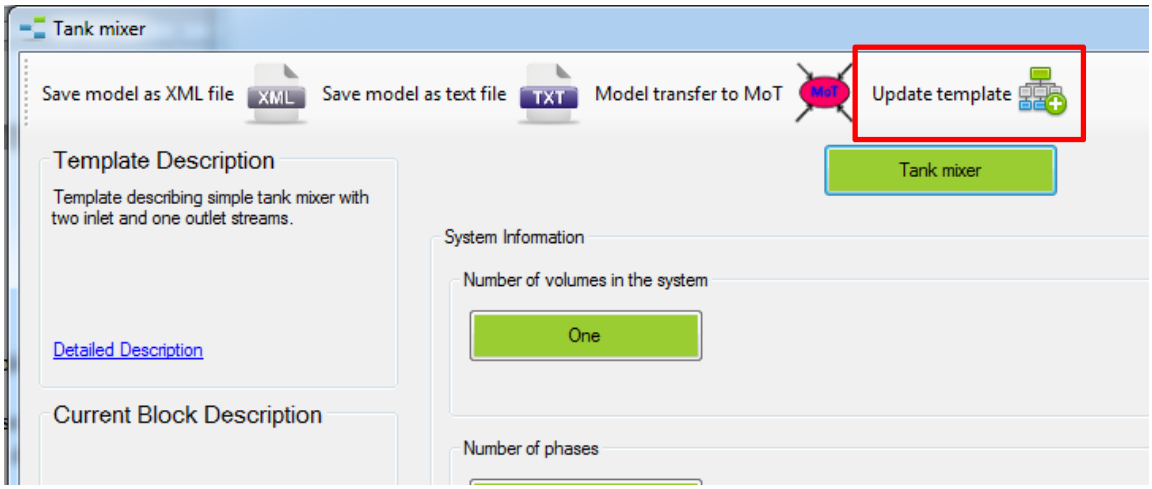

Figure 38. Update template button on the template screen.

Add new sub-layer in “System Information” layer – “Number of inlet streams” and add two blocks to it. First block will be for two streams and it will be default one, second block will be for three streams (See Fig. 39, 40, 41).

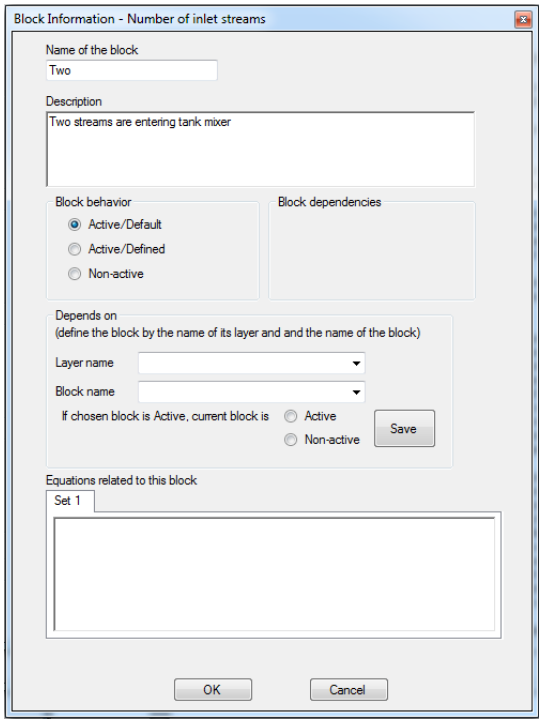

Figure 39. Information form for the first block

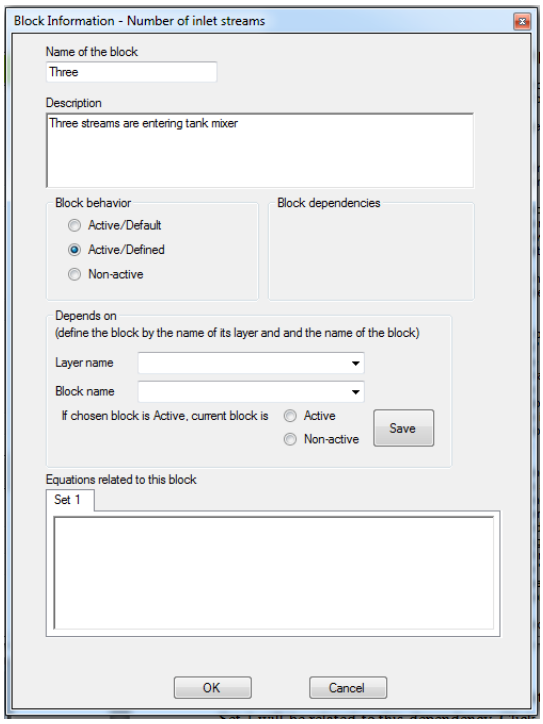

Figure 40. Information form for the second block

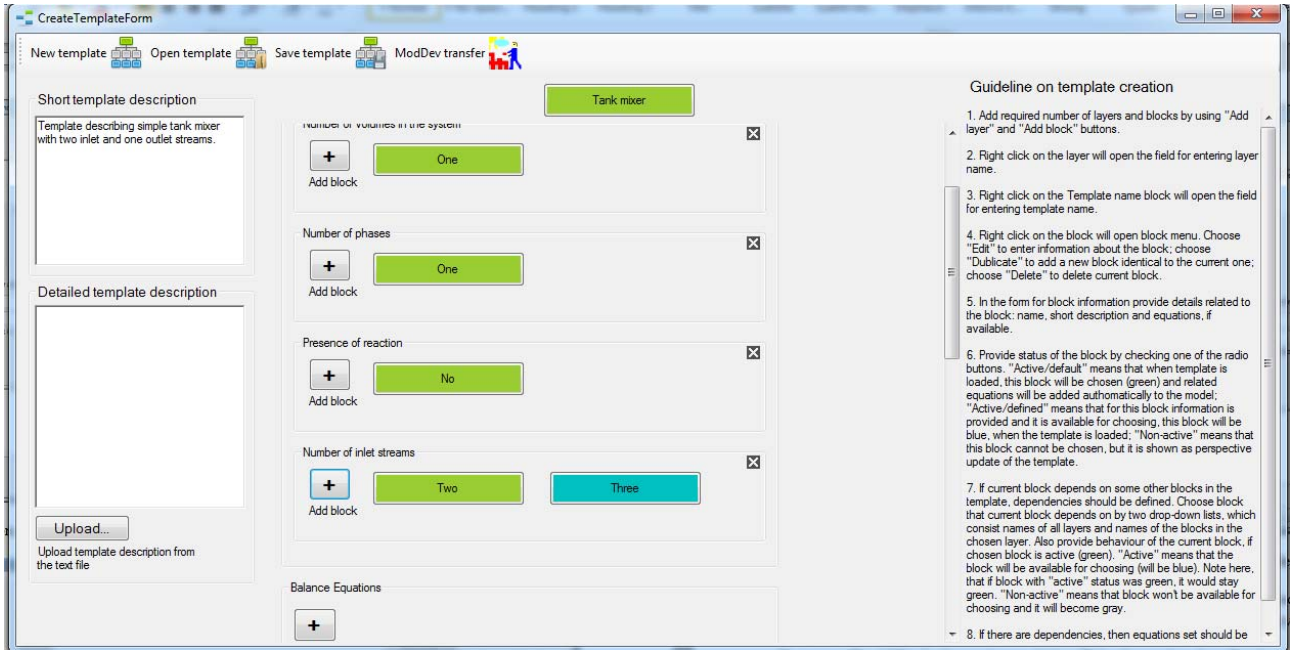

Figure 41. Template creation screen after adding new sub-layer for inlet streams.

Now we need to update equations in our template. Go to the “Steady State” block in “Mass balance” sub-layer and open its information form. Whether there are two inlet streams or more, we will still have steady state mass balance, but the equations should depend on the number of streams.

Therefore, we will define dependencies for this block. In the part of dependencies in the information form fill the name of sub-layer and the name of block from on which current block depends (Fig. 40). In our case – “Number of inlet streams” and “Two”.

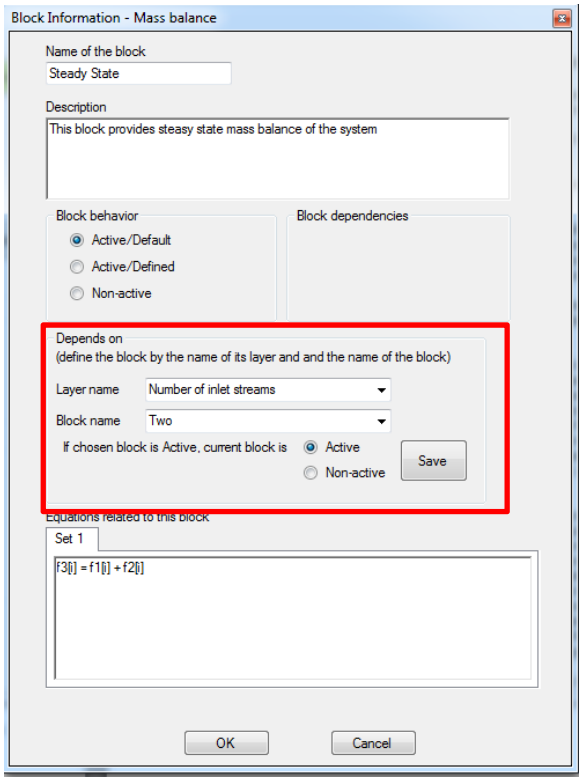

Figure 42. Describing dependencies.

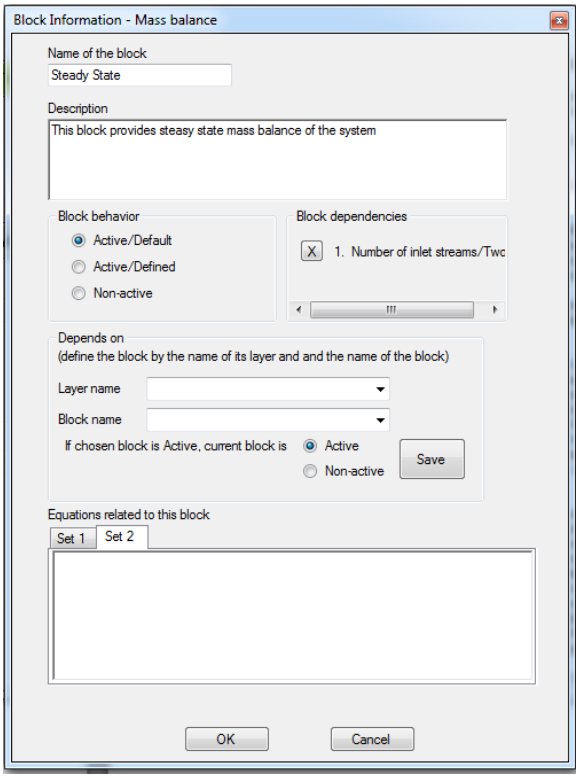

Figure 43. Saved dependency.

If chosen block is Active (green on the template use screen), then current block will be also active. Equations in Set 1 will be related to this dependency. Click “Save” button and dependency will be saved (Fig. 43).

Now we will add Set 2 of equations, which will be changed to describe three inlet streams. Also we will describe dependency of “Number of inlet streams”/”Three” block (Fig. 44). Close information form by clicking OK.

Similarly provide changes and dependencies for other block in layers “Balance Equations”, “Constitutive Equations”, “Connection Equations”. See Figures 45-47 for details.

Then we also need to correct template description, as it was related only to two inlet streams. After changing that we can save template (Fig. 48).

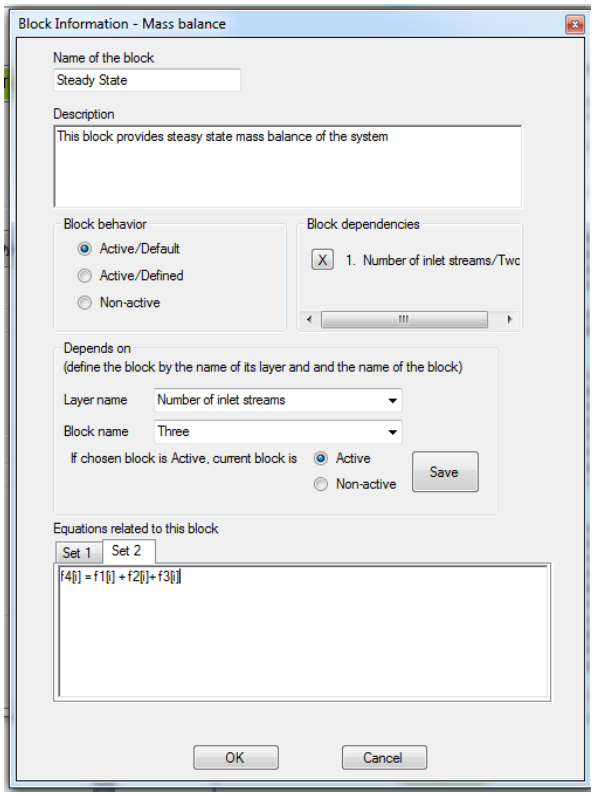

Figure 44. Describing second dependency.

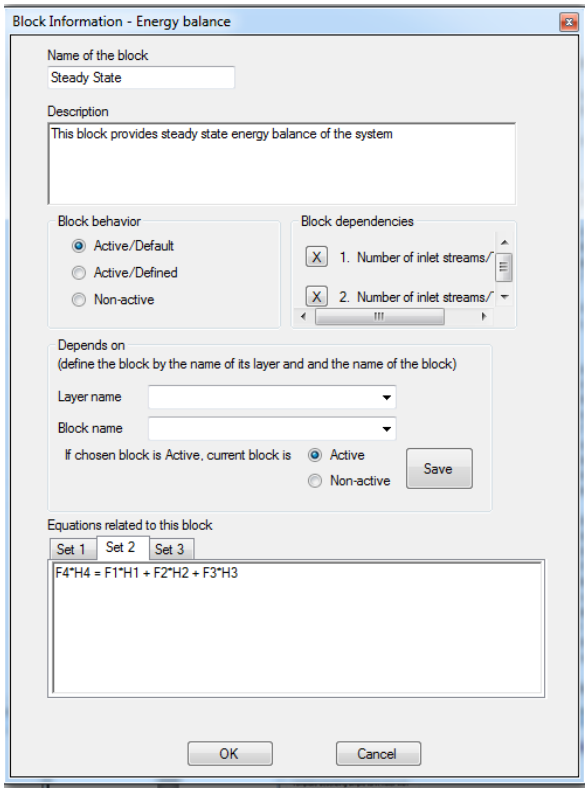

Figure 45. Dependencies for the energy balance.

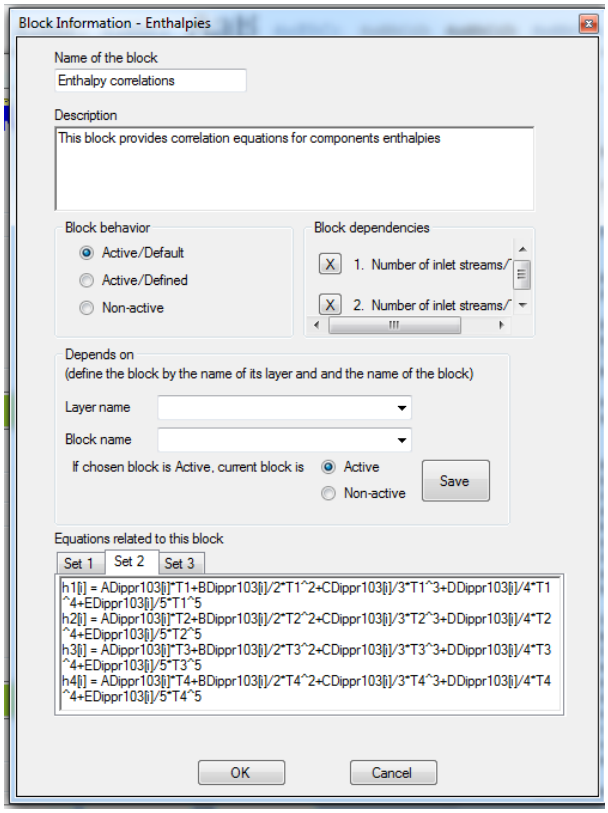

Figure 46. Dependencies for the enthalpies.

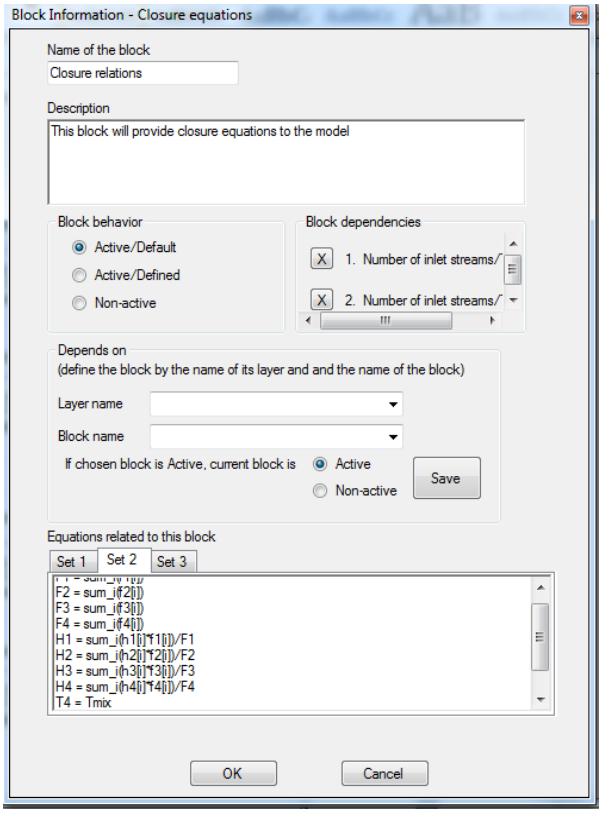

Figure 47. Dependencies for closure equations.

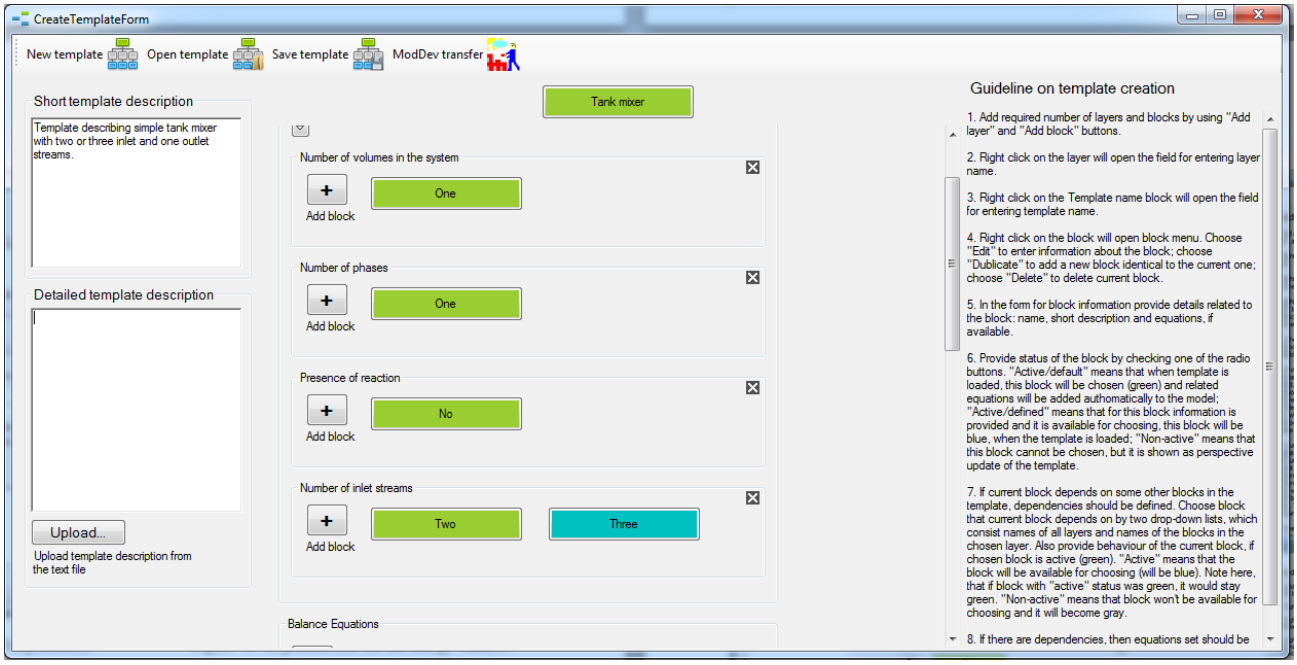

Figure 48. Template creations screen after updating template.

Now we will open our template from the starting screen again in order to check changes and dependencies (Fig. 49).

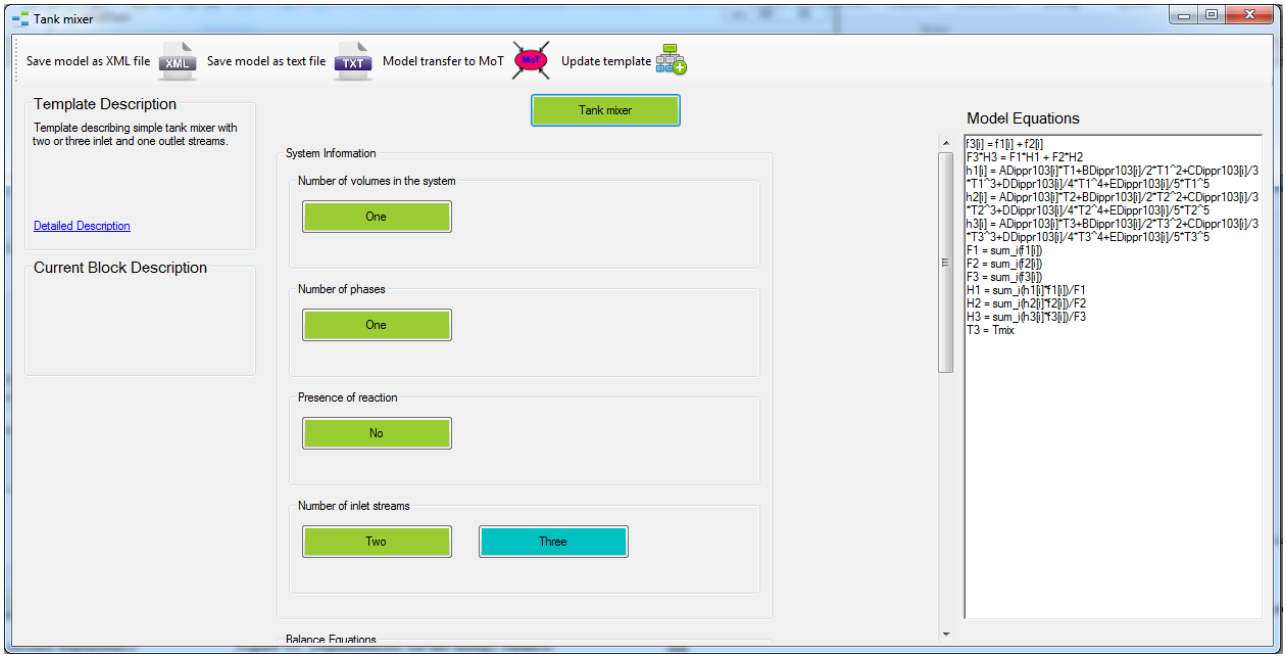

Figure 49. Template use screen of tank mixer template after updates.

Now we click on the blue block “Three” to show that we want to have three inlet streams in our model. It will become green and model equations will change accordingly. That means that our dependencies work fine.

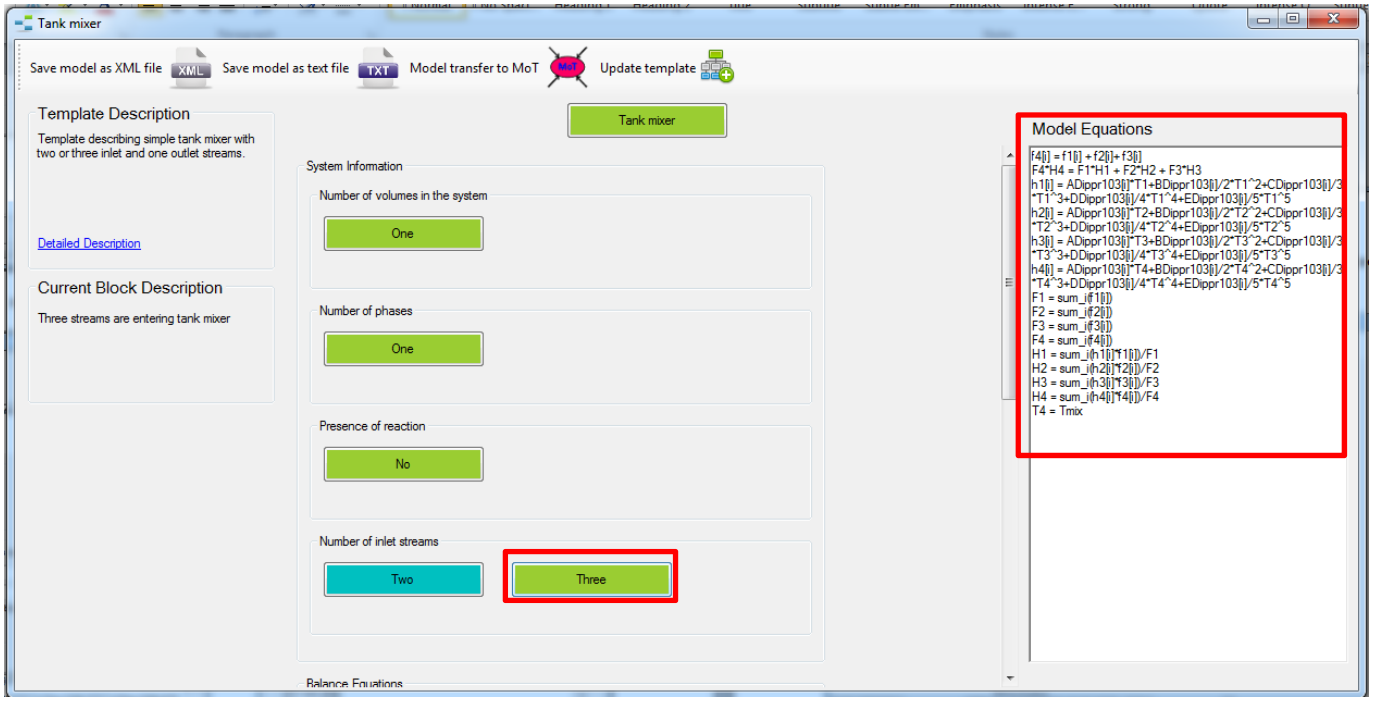

Figure 50. Template use screen of tank mixer template after updates.