Implementing MOSAIC Models in Aspen

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1   Introduction

This is a guide on how to export self-implemented models from MOSAIC to Aspen Custom Modeler and Aspen Plus in order to take advantage of Aspen's property data banks and integrate customized unit operation models into a flowsheet. Knowledge of modeling in MOSAIC and the use of functions, connectors and ports are pre-requisites. No knowledge of ACM language is required, but little knowledge on setting up a simulation in Aspen Plus is expected.

2   Creating a MOSAIC Model

The first step is to create a MOSAIC model as one normally would. In this example, an adiabatic two liquid stream mixer is to be simulated based on a MESHI equation system as described below:

$$0 = F^{in,I} \cdot x_i^{in,I} + F^{in,II} \cdot x_i^{in,II} - F^{out} \cdot x_i^{out} \tag{1}$$

$$0 = F^{in,I} \cdot h^{in,I} + F^{in,II} \cdot h^{in,II} - F^{out} \cdot h^{out} \tag{2}$$

$$\sum_{i=1}^{NC} x_i^{out} = 1 \tag{3}$$

$$0 = P^{in,I} - P^{out} - \Delta p^{out} \tag{4}$$

3   Introducing Function Calls

Aspen Custom Modeler has many built-in functions or procedures (as they are called in the program), for enthalpy, density, viscosity, fugacity, activity coefficient and etc. These are generic function calls, which are independent of

Table 1: ACM Enthalpy Function Applications

Generic Naming	Application I	Application II	Application II
h	$h^{I,in}$	$h^{II,in}$	h^{out}
p	$p^{I,in}$	$p^{II,in}$	p^{out}
x_i	$x_i^{I,in}$	$x_i^{II,in}$	x_i^{out}
θ	$\theta^{I,in}$	$\theta^{II,in}$	θ^{out}

the selected property package. The calculations will be performed according to the selected property package (NRTL, SRK, PENG-ROB, etc.) for every simulation . This allows easy model reutilization.

In this example, the enthalpy of the liquid streams is going to be calculated by an Aspen Custom Modeler procedure. As the enthalpy is a function of pressure, composition and temperature, the procedure has the following structure:

$$h(p, x_i, \theta) = ACMCalculateMolarLiquidEnthalpy \qquad (5)$$

Where h is the liquid molar enthalpy in GJ/kmol, p is the pressure in bar, x_i is the molar fraction of component i and θ is the temperature in C. Note that these units matter, since ACM cannot know which units are being used in the model. Additional equations for unit conversion may be necessary.

The MOSAIC function that generates this ACM procedure has already been implemented and can be loaded into the equation system with the following 3 applications, for each one of the streams:

4 Introducing Ports

Ports are necessary to allow the model to be connected to streams. Two inlet ports and one outlet port are necessary. Every port must have a connector to translate the variable names and an interface containing the required variables for the stream.

The interface containing the necessary variables has already been implemented an can be seen below.

Connectors need to be created following the nomenclature matching as following. It is not necessary to translate variables for molar volume as these variables are not included in the mixer model.

Figure 1: Interface for ACM Stream Connection

Table 2: Variable matching for the ports

Super Naming	Sub Naming I	Sub Naming II	Sub Naming II
θ	$\theta^{I,in}$	$\theta^{II,in}$	θ^{out}
F	$F^{I,in}$	$F^{II,in}$	F^{out}
h	$h^{I,in}$	$h^{II,in}$	h^{out}
p	$p^{I,in}$	$p^{II,in}$	p^{out}
x_i	$x_i^{I,in}$	$x_i^{II,in}$	x_i^{out}
v	-	-	-

Now the inlet and outlet ports can be created by selecting the direction and loading the interface and the connectors.

5 Code Generation

Open the newly created equation system in the **Evaluate** tab. At this point it should contain 4 equations, the enthalpy function with 3 applications and 3 external ports. Select the value for the index i (number of components) as 2 and confirm. In the **variable specification** tab, select the pressure drop (Δp^{out}), inlet streams' flows, compositions, temperature and pressure as design variables. The enthalpies of the three streams should appear in the calculated variables table, as they will be calculated by the function/procedure. Give proper starting values for the flow, composition, temperature and pressure of the outlet stream. An example of problem specification is given below:
   In the **evaluation** tab select ACM NLE Funcs to Equas in the language specification and press generate code. This code is now ready to be copied and compiled in Aspen Custom Modeler.

Table 3: Design Variables

Variable	Value	Units
Δp^{out}	0	bar
$\theta^{I,in}$	25	C
$F^{I,in}$	1	kmol/h
$p^{I,in}$	1.02	bar
$x_{i=1}^{I,in}$	1.0	kmol/kmol
$x_{i=2}^{I,in}$	0.0	kmol/kmol
$\theta^{II,in}$	25	C
$F^{II,in}$	1	kmol/h
$p^{II,in}$	1.02	bar
$x_{i=1}^{II,in}$	0.0	kmol/kmol
$x_{i=2}^{II,in}$	1.0	kmol/kmol

Table 4: Iteration Variables

Variable	Initial Value	Lower Bound	Upper Bound	Units
θ^{out}	25	-273.15	1.0E09	C
F^{out}	2	0	1.0E09	kmol/h
p^{out}	1.02	0	1E09	bar
$x_{i=1}^{out}$	0.5	0	1	kmol/kmol
$x_{i=2}^{out}$	0.5	0	1	kmol/kmol

6 Solution in Aspen Custom Modeler

6.1 Configuring the Component List

- Add description to start a new project in ACM.

- Which Aspen version has been used?

- Methanol must be named METHANOL and water as WATER

Open the ACM user interface. For this example we are using version 8.4. Before creating the model, it is necessary to configure a component list and a property package. In the **Model Explorer** select **Component List** and then double click on **Default**. Select the **use Aspen property system** option and click on **Edit using Aspen Properties**.
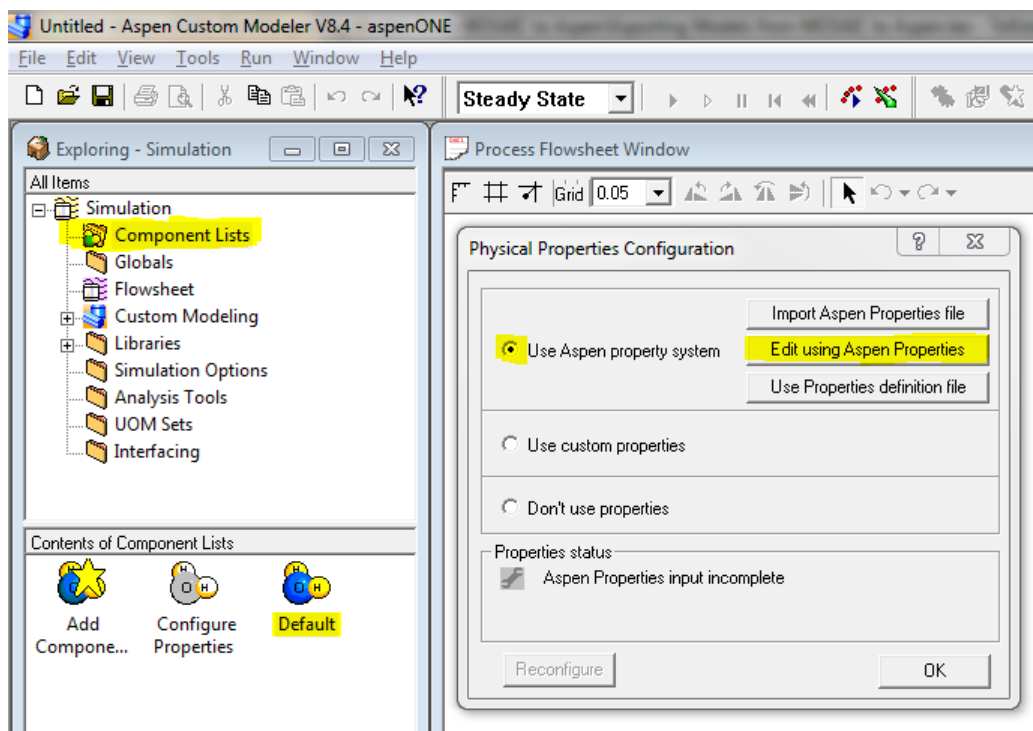
Figure 2: Configuring the Default Component List in ACM

This will initiate the Aspen Properties user interface. Here the component list and property methods can be specified normally as when starting an Aspen Plus simulation. In order to verify the non-ideal enthalpy calculations, a
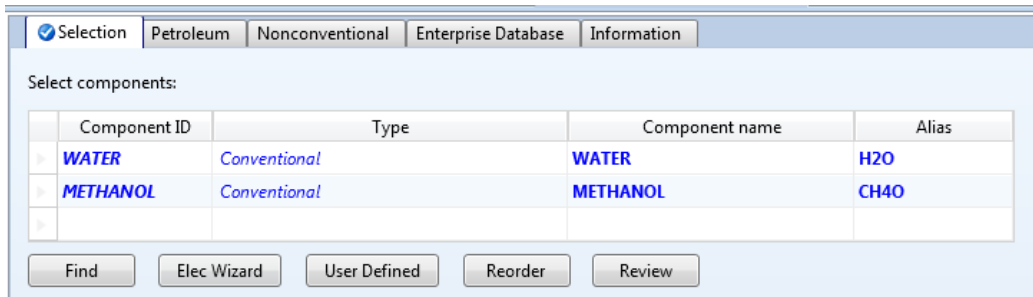
Figure 3: Component List in Aspen Properties

binary mixture of water and methanol will be used. Add water and methanol to the component list. It is essential to keep consistency in the component names, therefore the **Component ID** for water should be "WATER" and for methanol it should be "METHANOL".

Click **Next** (shortkey F4) to go to the **Methods** tab and select NRTL as the main property method.
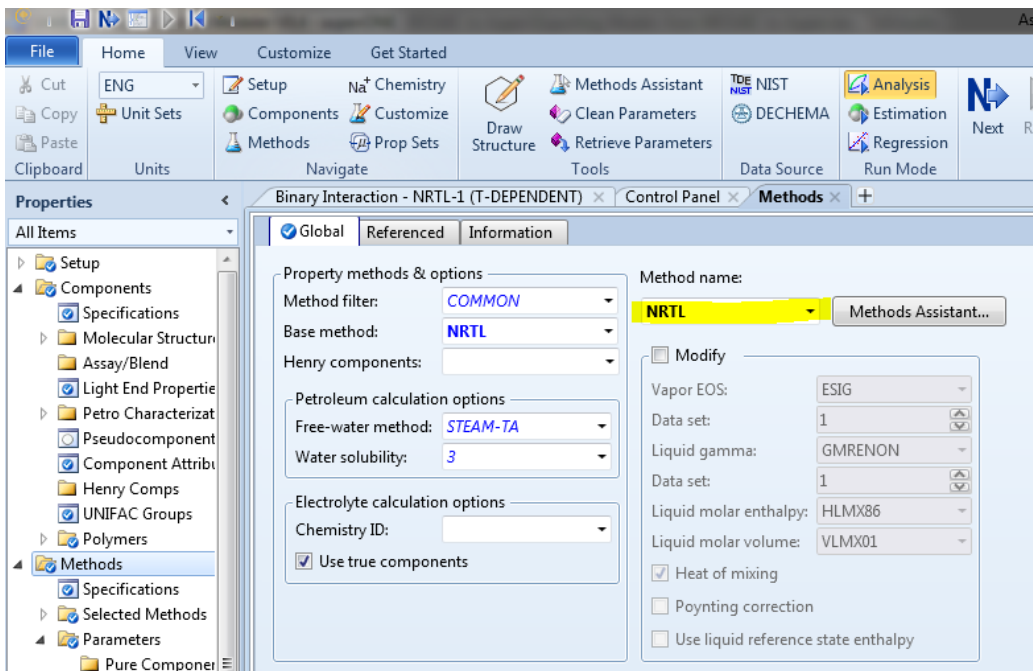

Figure 4: Component List in Aspen Properties

Click **Next** one more time to retrieve the binary interaction parameters and

again to run the property analysis. Once this is completed successfully, close the Aspen Property window and save the file when asked.

Back to the ACM window, it should be shown that the Component List setup was completed. Click on OK and add the available components to the ACM component list.

6.2   Creating a New Model

Now it is necessary to create a new model that will receive the code generated in MOSAIC. Again on the **Model Explorer** palette, select **Custom Modeling → Models** and then **Add Model** as highlighted below.
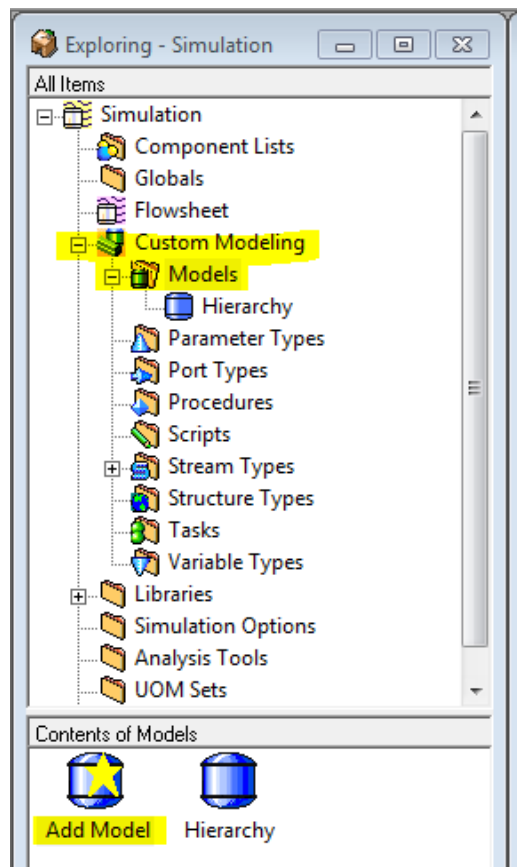

Figure 5: Adding a New Model in ACM

Name the model and paste the ACM code exported from MOSAIC in the

code window.

By default, the MOSAIC code generation will:

1. Name the model as mosaic_model

2. Name the component list as "prop"

3. Name components as "COMP1", "COMP2" and etc.

4. Name inlet ports as Feed1, Feed2 and etc.

5. Name Outlet ports as Prod3, Prod4 and etc.

The model name appearing on the code window must be the same as the name previously given, so change the fist line from mosaic_model to your given name. Comment or erase the line with the component list declaration to make ACM utilize the default component list as desired. The component names must match the ones in the component list. By using the tools "search for" and "replace" it is possible to replace "COMP1" and "COMP2" by "WATER" and "METHANOL".

One might also want to rename the ports to make it clear to the user where to connect the streams. In a distillation column, for example, it's advisable to rename the outlet ports as "Distillate" and "Bottom Product", rather than "Prod2" and "Prod3". This is not important for the mixer.

The default icon for all models generated in ACM is the flash vessel. It is possible to change this icon and design customized icons that reassemble the real equipment. Under the **Contents** of your model, there's an option to **Add Icon**.

Once these minor editions are done, right-click on the coding window and click on compile (shortkey F8). Compilation should be completed without any errors. Close the window containing the code. In the **Model Explorer** palette, click on the mixer model and drag it to the **Process Flowsheet Window** to add a mixer module to the flowsheet.

A light-green square on the lower right part of the ACM window indicates that the degree of freedom is zero and the simulation is ready to be executed. It would show a red arrow pointing upwards if the model is overspecified and pointing downwards if it is underspecified. Run the model by clicking on the run button in the upper part of the screen. Check the results.
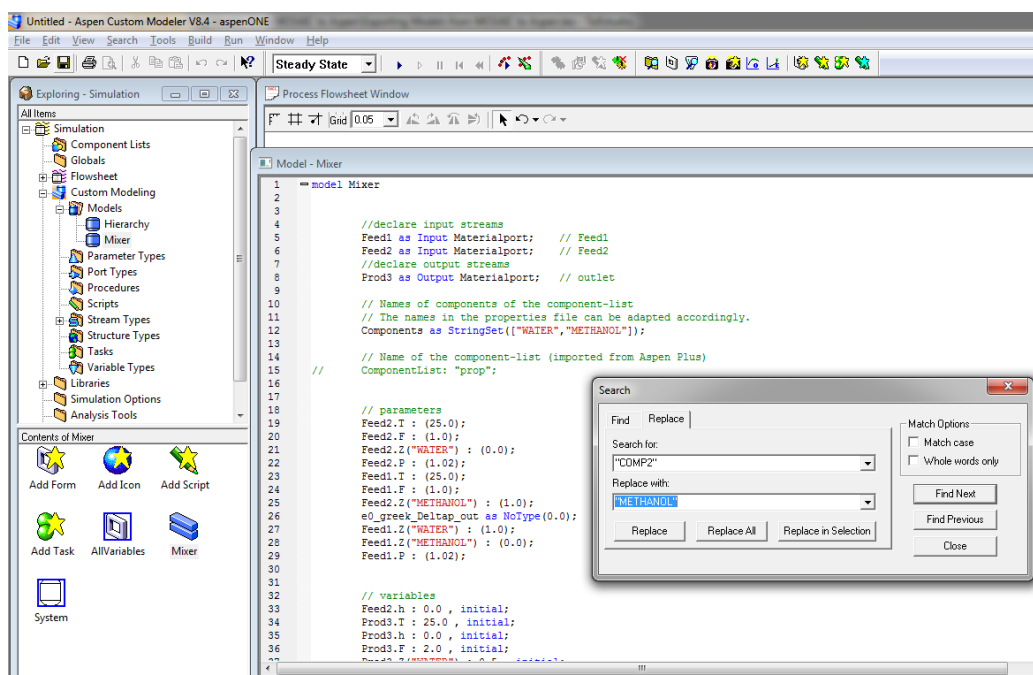
Figure 6: Coding Window in ACM

7 Exporting an ACM Model to Aspen Plus

Now the model is to be exported to Aspen Plus. For this exercise we are using Aspen Plus version 8.6. When simulating a unit in an Aspen Plus flowsheet, the inlet ports will be connected to streams. Streams in Aspen Plus already have a built-in function to calculate the enthalpy once pressure, composition and temperature are specified. This means that there is no need to calculate the enthalpies of the inlet streams using the function/procedure anymore. Therefore, these lines must be commented or deleted from the ACM code.

ADD: HOW TO OPEN AND EDIT THE CODE. FEED info can be retained as initials

It is necessary to have a proper version of Microsoft Visual Studio installed in order to perform the operation. It is possible to export to DLL, in order to generate a **.dll** file which can be read by Aspen Plus as a unit operation. It is also possible to export to MSI, which will generate a **.msi** file that can later be used to install the **.dll** file in any desired location.

In the **Model Explorer** right click on the model name and select **EXPORT TO MSI**. When asked "Do you want to install the model now?" click yes and follow the installation steps. Keep the default location for the file.

Once the file has been installed correctly, start a new Aspen Plus simulation
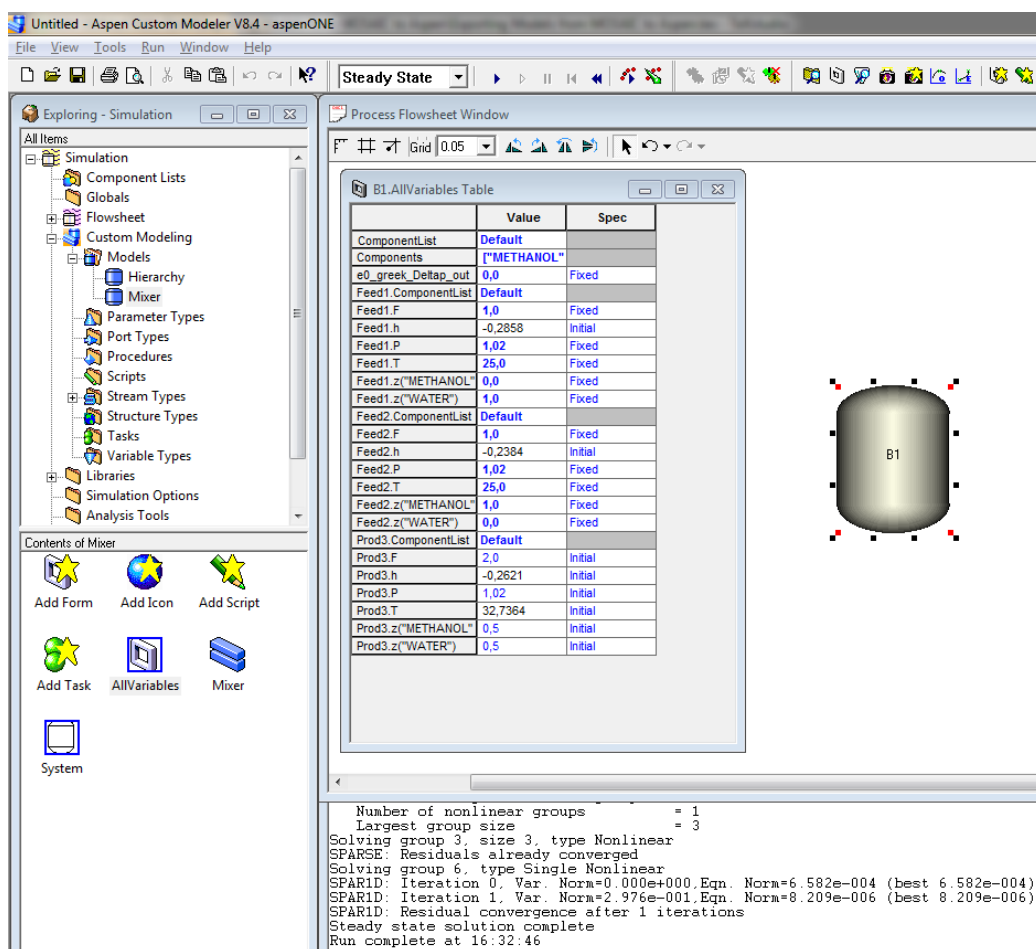
Figure 7: Flowsheet Simulation and Results

file, select water and methanol as components and NRTL as property package. Run a property analysis and then enter the simulation environment. To enable the ACM models to be shown in the **Model Palette**, select the tab **Customize** and then **Manage Libraries** and then activate the ACM Models.

Add the customized mixer model to the flowsheet and repeat the simulation done in ACM. The results should be the same.
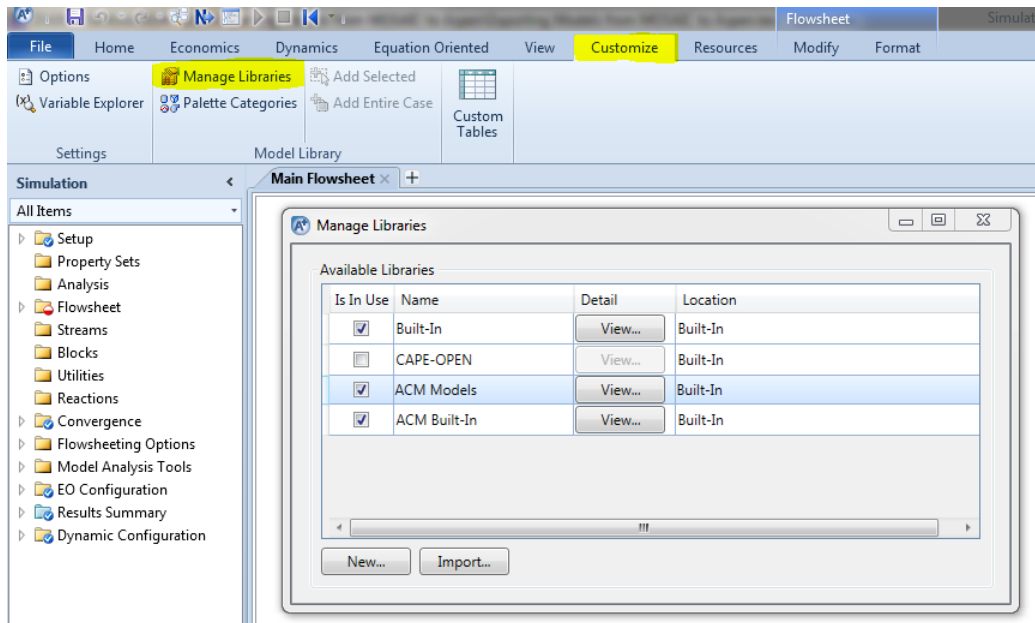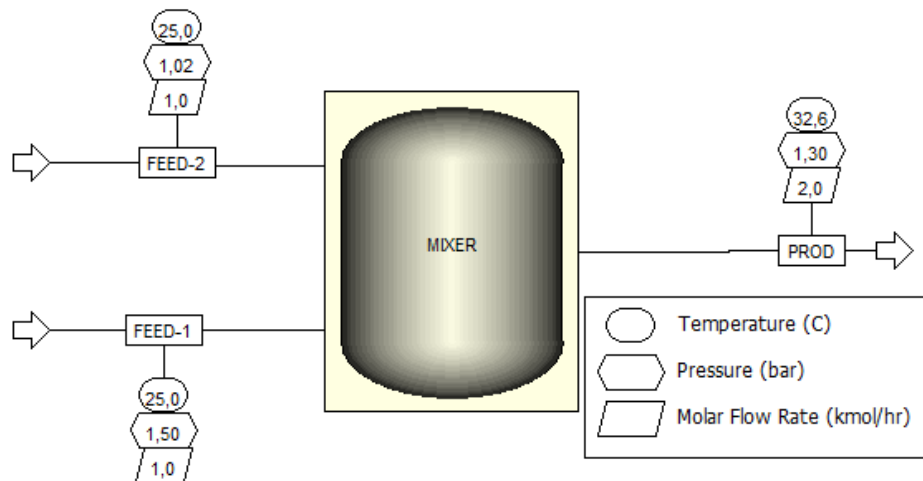
Figure 8: Enabling ACM Models in the Model Palette

Figure 9: Simulating the Mixer