APPLICATION EXAMPLE

SIMIT simulation of a stirred tank reactor with PCS 7

SIMATIC PCS 7 V9.1 SP2, SIMATIC SIMIT V11.0

SIEMENS
Legal information

Use of application examples
Application examples illustrate the solution of automation tasks through an interaction of several components in the form of text, graphics and/or software modules. The application examples are a free service by Siemens AG and/or a subsidiary of Siemens AG ("Siemens"). They are non-binding and make no claim to completeness or functionality regarding configuration and equipment. The application examples merely offer help with typical tasks; they do not constitute customer-specific solutions. You yourself are responsible for the proper and safe operation of the products in accordance with applicable regulations and must also check the function of the respective application example and customize it for your system.
Siemens grants you the non-exclusive, non-sublicensable and non-transferable right to have the application examples used by technically trained personnel. Any change to the application examples is your responsibility. Sharing the application examples with third parties or copying the application examples or excerpts thereof is permitted only in combination with your own products. The application examples are not required to undergo the customary tests and quality inspections of a chargeable product; they may have functional and performance defects as well as errors. It is your responsibility to use them in such a manner that any malfunctions that may occur do not result in property damage or injury to persons.

Disclaimer of liability
Siemens shall not assume any liability, for any legal reason whatsoever, including, without limitation, liability for the usability, availability, completeness and freedom from defects of the application examples as well as for related information, configuration and performance data and any damage caused thereby. This shall not apply in cases of mandatory liability, for example under the German Product Liability Act, or in cases of intent, gross negligence, or culpable loss of life, bodily injury or damage to health, non-compliance with a guarantee, fraudulent non-disclosure of a defect, or culpable breach of material contractual obligations. Claims for damages arising from a breach of material contractual obligations shall however be limited to the foreseeable damage typical of the type of agreement, unless liability arises from intent or gross negligence or is based on loss of life, bodily injury or damage to health. The foregoing provisions do not imply any change in the burden of proof to your detriment. You shall indemnify Siemens against existing or future claims of third parties in this connection except where Siemens is mandatorily liable.
By using the application examples you acknowledge that Siemens cannot be held liable for any damage beyond the liability provisions described.

Other information
Siemens reserves the right to make changes to the application examples at any time without notice. In case of discrepancies between the suggestions in the application examples and other Siemens publications such as catalogs, the content of the other documentation shall have precedence.
The Siemens terms of use (https://support.industry.siemens.com) shall also apply.

Security information
Siemens provides products and solutions with industrial security functions that support the secure operation of plants, systems, machines and networks.
In order to protect plants, systems, machines and networks against cyber threats, it is necessary to implement – and continuously maintain – a holistic, state-of-the-art industrial security concept. Siemens' products and solutions constitute one element of such a concept.
Customers are responsible for preventing unauthorized access to their plants, systems, machines and networks. Such systems, machines and components should only be connected to an enterprise network or the internet if and to the extent such a connection is necessary and only when appropriate security measures (e.g. firewalls and/or network segmentation) are in place.
For additional information on industrial security measures that may be implemented, please visit https://www.siemens.com/industrialsecurity.
Siemens' products and solutions undergo continuous development to make them more secure. Siemens strongly recommends that product updates are applied as soon as they are available and that the latest product versions are used. Use of product versions that are no longer supported, and failure to apply the latest updates may increase customer's exposure to cyber threats.
To stay informed about product updates, subscribe to the Siemens Industrial Security RSS Feed under https://www.siemens.com/icert.
# Table of contents

1. Simulation of a stirred tank reactor ................................................................. 5  
   1.1. Overview ........................................................................................................ 5  
   1.2. Components of a stirred tank reactor ........................................................... 7  
   1.3. Principle of operation .................................................................................... 9  
   1.4. Hardware and software components ........................................................... 10  

2. Preparation and commissioning with SIMATIC PCS 7 ........................................ 11  
   2.1. Preparations .................................................................................................. 11  
   2.1.1. Preparations of PCS 7 ............................................................................ 11  
   2.1.2. Preparations of SIMIT ......................................................................... 13  
   2.1.3. Preparations of the OS .......................................................................... 15  
   2.1.4. Downloading stations ............................................................................ 16  
   2.2. Operation .................................................................................................... 17  

3. Structure and principle of the SIMIT simulation ................................................. 19  
   3.1. Uniform project structure in PCS 7, PCS neo and SIMIT ............................ 19  
   3.2. Simulation structure in SIMIT ..................................................................... 21  
   3.3. Coupling (signal level) .............................................................................. 24  
   3.4. Device level ................................................................................................ 25  
   3.5. Simulation model structure ....................................................................... 27  
   3.5.1. Process level ......................................................................................... 27  
   3.5.2. Simulation of the inflows ....................................................................... 36  
   3.5.3. Simulation of the fill level ..................................................................... 37  
   3.5.4. Simulation of the pressure ..................................................................... 40  
   3.5.5. Simulation of the temperature ................................................................. 42  
   3.6. Parameters and overview .......................................................................... 48  

4. Fundamentals – Process Technology .................................................................. 49  
   4.1. Process simulation ...................................................................................... 49  
   4.2. Mass balance .............................................................................................. 52  
   4.3. Fill level ...................................................................................................... 53  
   4.4. Heat balance .............................................................................................. 54  
   4.5. Pressure ..................................................................................................... 58  

5. Appendix ........................................................................................................... 59  
   5.1. Service and support .................................................................................... 59  
   5.2. Links and literature .................................................................................... 60
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.3. Change documentation</td>
<td>60</td>
</tr>
</tbody>
</table>
1. Simulation of a stirred tank reactor

1.1. Overview

A PCS 7 project for a system grows in complexity due to the increasingly important requirement of availability and individuality of the system. For this reason, extensive tests are carried out to test the automation program. To make this possible one needs particular system states and responses from actuators and sensors with which one can check whether the automation program behaves correctly. The provision of responses or the system state is very laborious or not possible without a suitable tool.

For this reason, nowadays one can find tools such as SIMIT Simulation Framework (hereafter referred to as SIMIT), which simplify the simulation of signals, devices and process states in a significant way.

This application example describes how to use the SIMIT simulation software to easily and quickly create the required simulation for your PCS 7 project. A stirred tank reactor is used as a simulated unit. This is based on the "stirred tank reactor" PCS 7 Unit Template.

The technical description of the "stirred tank reactor" system section can be found in the documentation for the "stirred tank reactor" PCS 7 Unit Template. This is available in the following entry:

PCS 7 Unit Template "stirred tank reactor":

The following P&I flow chart is the basis for the configuration of all projects:
1.2. Components of a stirred tank reactor

This application example contains a sample implementation of a stirred tank reactor, which occurs as a subsystem in a wide variety of process engineering systems.

The stirred tank reactor contains the following main components in SIMATIC PCS 7 and SIMATIC Pcs neo, as well as in SIMIT:

1. Inflow of input materials with ratio control
2. Agitator
3. Pressure control
4. Temperature control (motor staging of the reactor temperature via the jacket temperature)
5. Reactor
6. Product discharge with level control

(1) Inflow of input materials

The input materials (reactants) are added to the vessel via the inflow and in a defined mixture ratio. The flow rate of the main components is predefined by means of a fixed setpoint and controlled by the master controller. Each further component receives a setpoint, which is proportional to the primary current of the master controller. This is, therefore, a ratio control which can also be used for other purposes which have nothing to do with the stirred tank reactor. A catalyst is also fed to the vessel in a defined flow rate as an additional input material.

(2) Mixer

The motorized mixer has the task of mixing the added input materials or components together and to create a uniform distribution of the material concentration and temperature within the reactor. To avoid damaging the mixer, the mixer must be disabled if the level falls below the defined filling level.

(3) Pressure control

For chemical reactions to take place, the pressure within the reactor must be constant. To meet this requirement, the pressure control maintains a preset vessel temperature and stabilizes pressure spikes on the fly. To increase the pressure, an inert gas (e.g., nitrogen) is supplied through a supply line. To reduce the pressure, an outlet valve is opened, thus allowing the gas mixture to escape from the vessel. This is a split range control and it can also be used for other applications (that have nothing to do with the reactor) where two actuators should be controlled by one controller.

(4) Temperature control

Another requirement for chemical reactions to take place is to have the reactants in the reactor (vessel) at the correct temperature. Due to the temperature dependency of the reaction speed and the exothermic or endothermic chemical reactions, reactor temperature control is a particularly demanding task. This requirement is met by using a stirred tank reactor with vessel jacket cooling and a diathermic partition. To achieve a specified temperature inside the reactor, the system feeds either hot steam or cooling water via supply lines into the vessel jacket. It is assumed that excess cooling water (e.g., from the overflow or pressure relief valve) is automatically released. The tank jacket influences the temperature inside the reactor with a small lag. Therefore, this is motor staging with one master controller for the reactor internal temperature and one slave controller (with split-range output) for the jacket temperature. Besides for the reactor, such a technical function can also be used for other task settings where the temperature is to be controlled indirectly via a service medium.

(5) Reactor

Chemical reactions take place in the reactor. The reactor is selected and designed considering sometimes complex process engineering interrelationships. These include:

- Reaction mixtures that require a special design or container properties
- Inflow and outflow volumes to determine the reactor size
- Reaction process in the environmental conditions required for this (Temperature and pressure)

(6) Product discharge

The flow rate of the product that will be discharged depends on the filling level of the reactor and is controlled in a way that the reactor’s filling level remains constant. Whenever there is a filling level change (due to differences between the
inflowing and outflowing volumes), the controller reacts to the filling level changes and adjusts them by either lowering or increasing the outflow volume.
1.3.  **Principle of operation**

From the entry pages of the application example, you can download the following projects:

- SIMIT simulation model "stirred tank reactor"
- PCS 7 project "stirred tank reactor"

The SIMIT project allows you to explore the operation, functionality, and benefits of SIMATIC PCS 7 or PCS neo from engineering to process control using a practical example. The simulation includes the most important devices and signals of a stirred tank reactor. In addition, you can use the simulation to generate desired process messages or simulate process behavior. The installation is modular and is based on physical principles.

---

**NOTE**

The SIMIT simulation of this application example is identical to the SIMIT project of the PCS neo application example "Stirred tank reactor". A description on how to connect the PCS neo project to the SIMIT simulation is available in this entry:

1.4. Hardware and software components

The following hardware and software components were used to create this application example:

<table>
<thead>
<tr>
<th>Components</th>
<th>Quantity</th>
<th>Article number</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIMATIC PCS 7 V9.1 SP2</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SIMIT SP V11.0</td>
<td>1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The listed components can be obtained from the Siemens Industry Mall, for example.

This application example consists of the following components:

<table>
<thead>
<tr>
<th>Components</th>
<th>File name</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIMIT project</td>
<td>93148023_StirredTankReactor_SIMIT_V11_0.simarc</td>
<td>Project archive</td>
</tr>
<tr>
<td>PCS 7 project</td>
<td>93148023_StirredTankReactor_PCS7V9_1_SP2.zip</td>
<td>Project archive</td>
</tr>
<tr>
<td>Documentation</td>
<td>93148023_StirredTankReactor_PCS7_V9_1_SP2_SIMIT_V11_0_en.pdf</td>
<td>This document</td>
</tr>
</tbody>
</table>

NOTE: The mentioned software versions are compatible to each other. The usage of older software versions is not possible. The usage of newer software versions is basically possible. Then, the compatibility has to be checked beforehand: [https://support.industry.siemens.com/cs/ww/en/view/64847781](https://support.industry.siemens.com/cs/ww/en/view/64847781)
2. Preparation and commissioning with SIMATIC PCS 7

2.1. Preparations

2.1.1. Preparations of PCS 7

Download the SIMIT repository and the PCS 7 repository from the download page of this entry:


1. Start SIMATIC Manager.
2. Retrieve the PCS 7 repository using the "Retrieve" function and then open it.
3. Open the Hardware Configuration of the OS station (OS01). In the network interface properties, enter the IP address and MAC address of the host computer.

4. Compile and save the HW Configuration of the OS.
5. Compile the OS project with the changed IP settings.
6. Open the Hardware Configuration of the AS Station (VC01). You may enter any MAC address and an IP address in the properties of the network interface of the CP 443-1 (X1) that is in the same IP range as the host computer.
NOTE

For the operation of the SIMIT VC (Virtual Controller), it is additionally necessary to enter the IP address of the AS Station in the network settings of the host computer.

7. Compile and save the HW Configuration of the AS.
8. Change the PG/PC interface in the SIMATIC Manager to obtain access to the VC. Therefor, navigate to "Options > Set PG/PC Interface..." in the menu bar and select the respective network interface. In this application example, the interface "Intel(R) 82574L Gigabit Network Communication.TCP/IP.1" was used.
2.1.2. Preparations of SIMIT

1. Start SIMIT.
2. Retrieve the SIMIT archive "109783866_StirredTankReactor_SIMIT_V10_3.simarc" with the "Retrieve" function and then open the project.
3. Open the Project manager and navigate to the property "Engineering". Delete the entries in the properties "Server" and "Project".

4. Create a new Virtual Controller coupling. The signal table is imported from the PCS 7 project "StirredTankReactor_MP". This creates all the relevant signals.

5. After the import, check the active address of the VC. Only the IP address that is also parameterized in the Windows network settings should be selected.
6. Start the simulation Runtime. This also starts the Virtual Controller.
2.1.3. Preparations of the OS

1. In the component view in the SIMATIC Manager right-click on the OS and select the menu option "Open object". The WinCC Explorer is started.
2. Confirm the "Configured server not available" dialog with "OK".
3. In WinCC Explorer, open the properties of your computer and, in the opened "Computer properties" dialog, click on the "Use Local Computer Name" button.
4. Confirm the "Change computer name" message with "OK".
5. In the WinCC Explorer, click on "File > Exit" and in the subsequent dialog select "Terminate WinCC Explorer and close project".
6. Then confirm with "OK".
7. Right-click on the OS and select "Translate" from the menu, then continue clicking until you reach the "Network Connections" window.
8. Check that the correct connection has been selected and that the WinCC unit "TCP/IP" is selected.
9. Compile the OS.
10. Reopen the WinCC Explorer as described in step 1.
11. Open by double-clicking on "Variables library".
12. Right-click on the TCP/IP interface and set the network interface in the tab "Unit" according to the used network interface.
13. Close the "Variables library".
2.1.4. **Downloading stations**

Switch back to PCS 7 and perform the following operations:

1. Load the hardware configuration into the VC.
2. Load the AS program into the VC.
3. Open the OS project and start the OS runtime.
2.2. Operation

Initialization

A sequence is prepared to initialize the continuous process. Execute the sequence "StartReactor" once after starting the OS runtime.

Wait until the sequencer has run through the "RUNNING" sequence. After that, all setpoints can be adjusted via the controller blocks. The stop command in the sequencer starts the sequence "SHUTDOWN" to end the continuous operation.

1. Opening the sequencer in the faceplate
2. Start initialization
3. When the "RUNNING" sequence has been processed, the system is in continuous operation.
Operation

In continuous operation, you can monitor production and adjust target values if necessary.

1. Set point for total feedstock inflow (0–1000 L/h)
2. Ratio of component 1 in factor 0–0.4
3. Ratio of component 2 in factor 0–0.4
4. Set point for the inflow of the catalyst (0–200 L/h)
5. Reactor temperature setpoint (0–100°C, master controller for the heating jacket temperature controller)
6. Setpoint of the reactor content (0–100%)
7. Setpoint of the reactor pressure (0–10 bar)
8. Production and consumption data (KPI)

Shutdown

You can stop the continuous process by using the "SHUTDOWN" sequence. To do this, execute the "Stop" command (1) in the sequencer.
3. Structure and principle of the SIMIT simulation

Below you can find descriptions regarding the design of the project and the transformation of the individual physical models in SIMIT.

3.1. Uniform project structure in PCS 7, PCS neo and SIMIT

The hierarchy levels of SIMATIC PCS 7, SIMATIC PCS neo and SIMIT are structured in the same way. All projects contain the following hierarchy folders:

- Mixing (Agitation): Mixing of the product
- Inflow (Feed): Inflows to the reactor
- Level control (Level): Level control via the outflow
- Pressure control (Pressure): Control of the vessel pressure
- Temperature control (Temperature): Control of the reactor temperature
The present SIMIT project consists of the following components:

1. Coupling
2. Devices
3. Process
4. Parameters and overview
### 3.2. Simulation structure in SIMIT

The simulation model is the basis for testing the SIMATIC PCS 7 automation project. The simulation contains the main physical processes, devices, and signals of a stirred tank reactor. The installation is modular and is based on physical principles.

![Simulation Graph](image)

The "stirred tank reactor" simulation example includes several prefabricated, unified, and ready-connected device and process simulations. Using this sample solution as a basis, numerous instances with different parameterizations can be generated with adapted characteristics to be widely integrated in simulation solutions.

A simulation usually consists of 3 levels:

1. **Signal level**

   The signal level is mapped in SIMIT in the coupling. All signals necessary for communication with the automation system are created there. The coupling must be created correspondingly for the system used. The signals are then imported from the process control system.
2. Device level

Within the device level, all devices such as drives, valves, and measurement points are mapped. These models provide the AS with the necessary responses, such as when the motor has started, as well as valve positions or process values.

The following figure shows the simulation of an analog valve as an example.

1. Output signal (green) of the AS
2. Normalization of a raw value into a process value
3. Calculation of the operating time of the valve ("MonTiDynamic")
4. Behavior simulation
5. Normalization of a process value into a raw value
6. Peripheral connector "Input" (red) and global connectors for further processing

The devices are created using the components offered by SIMIT. SIMIT offers components that are adapted to the drive function blocks of the "Advanced Process Library".

Devices can be created manually or using the SMD import function. Using the SMD import, the data that is exported by the import export assistant from the automation project is combined with the valve and motor templates. The templates can be adapted to the respective application.
3. Process level

In SIMIT, the process level represents the physical behavior of the system. All physical parameters, such as temperatures, pressures, flows, and levels, are calculated here.

The physical processes in this application example are created using components from the standard library. The values to be processed are delivered by simulated devices, signals, other processes or are constants. The calculation results are forwarded to devices, signals or other processes using global connectors.
### 3.3. Coupling (signal level)

Within the coupling of SIMIT, all signals that are necessary for the communication between virtual AS and SIMIT are generated.

When creating the coupling, it is possible to import the signals from the HW Configuration of the PCS 7 or the PCS neo project. The import creates all signals with the hardware address, symbolic name, and data type. In this sample project, the normalization of the analog signals is performed within the device level charts.

When the simulation is active, you can read and change the current signal values in the coupling editor.

1. Current or manipulated values of the signals
2. Symbolic signal names
3. Hardware address
4. Data type
### 3.4. Device level

For each device or measurement point, a separate diagram is created in the corresponding hierarchy folder. The structure of the diagrams is the same for all valves, drives, and measurement points, except for the connected signals.

Corresponding templates are created in the project library in the "Templates > User Templates" area.

---

**Simulation of a valve**

The figure below shows the structure of the YC_Product diagram. This diagram helps simulating the reactor's outlet control valve.

![Diagram of YC_Product](image)

The diagram consists of the following components:

1. "Output" peripheral connector
   - Output signal of the AS: "Set position of the valve"

2. Process value scaling
   - Normalization of a raw value into a process value

3. "MUL" multiplication
   - Defines the operating time of the valve (half of the monitoring time "MonTiDynamic")

4. "DriveV4" type valve drive

5. Process value scaling
   - Normalization of a process value into a raw value

6. Peripheral connector "Input" (red) and global connectors for further processing

The peripheral connector output is connected to the signal "YC_Product_MV". In the device simulation, the manipulated variable, which is predefined by the automation system for the valve, is read through it.

The multiplier allows the predefinition of time, which should be required for opening and closing operation. In the application example, half of the monitoring time is spent on the valve block in the automation system.

The "DriveV4" valve drive tracks the analog input value continuously. Tracking is performed depending on the set opening or closing time ($T_{Open}$ or $T_{Close}$).

The outputs of the valve drive can be connected to the inputs of global connectors and peripheral connectors. The peripheral connectors forward the simulated values (valve position, end positions) to the automation system. The global connectors serve to provide the simulated valve values to other diagrams, e.g. to calculate the current flow through a valve.
Simulation of a motor

The following figure shows the structure of the "NS_StirringMotor" diagram. This diagram helps simulating the drive of the reactor's mixing motor.

![NS_StirringMotor Diagram](image)

The diagram consists of the following components:

1. "Output" peripheral connector
   - Output signal of the AS: "Start signal of the engine"

2. "MUL" multiplication
   - Defines the start and stop time of the motor (Half of the monitoring time "MonTiDynamic")

3. "DriveP1" type pump drive

4. Peripheral connector "Input" (red) and global connectors for further processing

The peripheral connector "Output" is connected to the signal "NS_StirringMotor_CTR". In the device simulation, the starting command from the automation system is read through it and interconnected with the latter. The multiplier allows the predefinition of time, which should be required for the acceleration and deceleration from standstill to the rated speed and back. In the application example, half of the monitoring time is spent on the motor block in the automation system.

The pump drive simulates the starting and stopping of the motor. The response signals are connected to the global connectors and the "Input" peripheral connector. The peripheral connector "Input" is connected with signal "NS_StirringMotor_FBR" and passes on the response to the automation system regarding whether the motor is running. The simulated values can be forwarded to other diagrams via the global connectors.

Simulation of a measurement point

The following figure shows the structure of the "FIC_Quantity" diagram. This diagram is used to simulate the inflow of the main component to the reactor. Since the value is calculated directly by the process simulation, only the normalization and the transfer of the raw value to the AS is done in this plan.

![FIC_Quantity Diagram](image)

1. Global connector – process value from process simulation
2. Normalization of a process value into a raw value
3. Input connector of the AS – transfer of the process value to the AS
3.5. Simulation model structure

3.5.1. Process level

The process level also has the same hierarchical structure as the device level. The process level contains the simulations of temperatures, pressures, volume flows and the fill level of the stirred tank reactor.

A diagram is created in the corresponding hierarchy folder for each value to be simulated. Macros have been created for repetitive calculations such as volume and heat flows. These can be used as often as needed, which leads to a significantly reduced configuration effort.

Macros

The following macros are provided and used in this application example:

- "Heat_Flow_1"
- "Heat_Flow_2"
- "Heat_Capacity"
- "PerHoutToPerSecond"
- "PerSecondToPerHour"
- "Rate_of_temperature_change"
- "Flow"
- "T_Mean"
"HeatFlow"

The "Heat_Flow" macro calculates the heat flow generated from an inflowing medium.

The following describes the structure of the macro:

The macro has the following input variables:

- "currentMassFlow" [kg/s] (current mass flow)
- "specificHeatCapacity" [m²/s²*K] (specific heat capacity of the inflowing medium)
- "Temp1" [K] (temperature of the inflowing medium)
- "Temp2" [K] (temperature of the reactor contents)

The output variable of the macro is the current heat flow "currentHeatFlow" [kg*m²/s³], which results from the temperature difference between the reactor contents and the inflowing medium.

The heat flow is calculated from the product of the corresponding mass flow, the specific heat capacity and the temperature difference.
"HeatExchange"

The "HeatExchange" macro is used to calculate the heat flow that results from the heat transfer between the reactor and the cooling jacket.

The figure below shows the structure of the macro:

The macro has the following input variables:

- "HeatTransferCoefficient" [kg/s³*K] (Heat transfer coefficient)
- "ContactArea" [m²] (Heat transfer area)
- "Temp1" [K] (Reactor temperature)
- "Temp2" [K] (Average cooling jacket temperature)

The output variable of the macro is the current heat flow "currentHeatFlow" [kg*m²/s³], which results from the temperature difference between reactor temperature and average cooling jacket temperature.

The heat flow is calculated from the product of the heat transfer coefficient, heat transfer area and temperature difference.
"Heat_Capacity"

The "HeatCapacity" macro calculates the specific heat capacity of a medium at a specific temperature.

The figure below shows the structure of the macro:

```
<table>
<thead>
<tr>
<th>Input Variables</th>
<th>Output Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>specificHeatCapacityRefTemp [m²/s²*K]</td>
<td>specificHeatCapacityCurrentTemp [m²/s²*K]</td>
</tr>
<tr>
<td>TempCoefficient [m²/s²*K²]</td>
<td></td>
</tr>
<tr>
<td>CurrentTemp [K]</td>
<td></td>
</tr>
<tr>
<td>RefTemp [K]</td>
<td></td>
</tr>
</tbody>
</table>
```

The macro has the following input variables:

- "specificHeatCapacityRefTemp" [m²/s²*K] (Specific heat capacity of the resource at reference temperature)
- "TempCoefficient" [m²/s²*K²] (Temperature coefficient of the medium)
- "CurrentTemp" [K] (Temperature of the medium)
- "RefTemp" [K] (Reference temperature)

The "specificHeatCapacityCurrentTemp" output of the macro is the specific heat capacity of the medium at the current temperature of the medium [m²/s²*K²].

The specific heat capacity at the current temperature is calculated from the sum of the specific heat capacity at a reference temperature and the product of the temperature coefficients and the difference between the process temperature and the reference temperature.
"PerHourToPerSecond"

The "PerHourToPerSecond" macro converts the flows from "per hour" into "per second" (e.g., volume flow m³/h to m³/s).

The figure below shows the structure of the macro:

The input of the macro uses the "PerHour" unit (current per hour). The macro converts current per hour into current per second or current per minute by dividing the value by 3600 or 60.

The macro has the following two outputs for the converted values:

- "PerSecond" (current per second)
- "PerMinute" (current per minute)

An unused output can be set to invisible.
"PerSecondToPerHour"

The "PerSecondToPerHour" macro converts the flows from per second into per hour (e.g., m³/h in m³/h).

The figure below shows the structure of the macro:

The input of the macro uses the "PerSecond" unit (current per second). The macro converts this value into per hour or per minute by multiplying it by 3600 or 60.

The macro has the following two outputs for the converted values:

- "PerHour" (current per hour)
- "PerMinute" (current per minute)

An unused output can be set to invisible.
"Rate_of_temperature_change"

The "Rate_of_temperature_change" macro calculates the temperature change for each time unit (e.g., K/s).

The figure below describes the structure of the macro:

The macro has the following inputs:

- **Heat_Flow** [kg*m²/s³]
  
  (heat flow in the reference area)

- **"Mass"** [kg]
  
  (Mass in reference space)

- **"specific_Heat_Capacity"** [m²/s²K]
  
  (specific heat capacity of the cover fabric)

The "rate_of_temp_change" output of the macro is the temperature change of the medium [K/s].

The temperature change is calculated by dividing the heat flow by the product of the mass in the reference area and the specific heat capacity of the reference material.
"Flow"

The "Flow" macro calculates the current flow rate through a valve with equal percentage characteristic (e.g., m³/h).

The figure below describes the structure of the macro:

```
The macro has the following inputs:

- "currentValvePosition" [%] (current valve position)
- "maxFlow" (Maximum flow rate with valve fully open)

The "currentVolumeFlow" output is the current flow rate (e.g., m³/h). The current flow rate is calculated from the product of the maximum flow rate and the square of the division of the current valve position by 100.
```
"T_Mean"

The "T_Mean" macro calculates the mean temperature in the cooling jacket. The figure below describes the structure:

The macro has the following inputs:

- "Heating" [K] (Temperature of the heating medium)
- Cooling [K] (Temperature of the coolant)
- TicJacket [K] (Temperature of the cooling jacket output)

The "TMean" output is the mean temperature of the cooling jacket.

The macro contains three calculations for the temperature:

- Mean value from the temperature of the heating medium and the temperature of the cooling jacket output
- Mean value from the temperature of the coolant and the temperature of the cooling jacket output
- Mean value from the temperature of the heating medium, the temperature of the coolant and the temperature of the cooling jacket output

Thanks to comparative and logical operators, the macro checks if heating or cooling is in progress or none of them. Based on the result of this test, the corresponding mean value is switched through to the output. The through-connection is done via a multiplexer.
3.5.2. Simulation of the inflows

The simulation project of the stirred tank reactor contains the following inflows:

- "Quantity" (inflow of the main component)
- "Comp1" (inflow of the secondary component 1)
- "Comp2" (inflow of the secondary component 2)
- "Catalyst" (inflow of the input material catalyst)

The structure of the simulation of the individual inflows differs only in the interconnected signals. The following figure describes an example of the structure of the diagrams at the inflow of the main component:

The global connector "YC_Quantity/Y1" passes the current valve position from the diagram "YC_Quantity" to the diagram "Quantity". The connector is connected to the "Flow" macro. The current flow is calculated based on the valve position and the maximum flow rate of 1000 l/h of the main component's inflow.

The current flow rate is passed on to the automation system with peripheral connector input "FIC_Quantity_PV". Furthermore, the flow rate is converted from l/h to m³/h (multiplication by 10⁻³) to make the current flow rate available for further calculations in other diagrams via the global connector "YC_Quantity/Flow".
3.5.3. **Simulation of the fill level**

In the present application example, the fill level simulation is accomplished in the "Level" and "Product" diagrams.

**"Product"**

The "Product" diagram simulates a discharge. In principle, the diagram structure corresponds to an inflow.

The figure below describes the structure of the "Product" diagram:

![Volume flow product diagram](image)

Compared to the structure of the diagrams for the inflows, only the peripheral connector "Input" is missing.

**"Level"**

The current fill level is calculated in the "Level" diagram, based on the incoming and outgoing flows. Different values, such as mass in the reactor [kg] or volume in the reactor [l] are also calculated.

The figure below describes the structure of the "Level" diagram:

![Level diagram](image)

The diagram is divided into the following 7 areas:

1. Feed
2. Discharge
3. Calculation of the current mass in the reactor
4. Total amount of the product for key performance
5. Calculation of the upper limit of integration
6. Conversion of mass to fill level in liters and percent
7. Sum of the current fill level and uniformly distributed noise to ± 1%
The following table contains the descriptions for each area:

<table>
<thead>
<tr>
<th>Area</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Feed</td>
</tr>
<tr>
<td>2</td>
<td>Discharge</td>
</tr>
<tr>
<td>3</td>
<td>Calculation of the current mass in the reactor</td>
</tr>
<tr>
<td>4</td>
<td>Total product mass</td>
</tr>
<tr>
<td>5</td>
<td>Calculation of the upper limit of integration</td>
</tr>
<tr>
<td>6</td>
<td>Conversions</td>
</tr>
<tr>
<td>7</td>
<td>Fill level with measurement noise</td>
</tr>
</tbody>
</table>

Global connectors
The following table summarizes the global connectors of the "Level" diagram, which forwards the values to other diagrams:

<table>
<thead>
<tr>
<th>Connector</th>
<th>Value</th>
<th>Charts</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;Catalyst_Flow_kg/h&quot;</td>
<td>Mass flow of the catalyst ([\text{kg}/\text{h}])</td>
<td>&quot;Density&quot;, &quot;Heat Capacity&quot;, &quot;Temp_Reactor&quot;</td>
</tr>
<tr>
<td>&quot;Comp1_Flow_kg/h&quot;</td>
<td>Mass flow of the secondary component 1 ([\text{kg}/\text{h}])</td>
<td>&quot;Density&quot;, &quot;Heat Capacity&quot;, &quot;Temp_Reactor&quot;</td>
</tr>
<tr>
<td>&quot;Comp2_Flow_kg/h&quot;</td>
<td>Mass flow of the secondary component 2 ([\text{kg}/\text{h}])</td>
<td>&quot;Density&quot;, &quot;Heat Capacity&quot;, &quot;Temp_Reactor&quot;</td>
</tr>
<tr>
<td>Connector</td>
<td>Value</td>
<td>Charts</td>
</tr>
<tr>
<td>----------------------------</td>
<td>-----------------------------------------------</td>
<td>---------------------------------</td>
</tr>
<tr>
<td>&quot;Quantity_Flow_kg/h&quot;</td>
<td>Mass flow of the main component [kg/h]</td>
<td>&quot;Density&quot;, &quot;Heat Capacity&quot;, &quot;Temp_Reactor&quot;</td>
</tr>
<tr>
<td>&quot;SL/SumFlowFeed*&quot;</td>
<td>Total mass flow of the inflows [kg/h]</td>
<td>&quot;Density&quot;, &quot;Heat Capacity&quot;, &quot;Connections*&quot;</td>
</tr>
<tr>
<td>&quot;SL/SumProduct*&quot;</td>
<td>Total product mass [kg]</td>
<td>&quot;Connections*&quot;</td>
</tr>
<tr>
<td>&quot;Mass_Reactor*&quot;</td>
<td>Mass of the reactor contents [kg]</td>
<td>&quot;Temp_Reactor*&quot;</td>
</tr>
<tr>
<td>&quot;Volume_Reactor*&quot;</td>
<td>Volume of the reactor contents [m³]</td>
<td>&quot;Pressure*&quot;</td>
</tr>
<tr>
<td>&quot;SL/MReactorLiter*&quot;</td>
<td>Volume of the reactor contents [l]</td>
<td>&quot;Connections*&quot;</td>
</tr>
<tr>
<td>&quot;SL/MReactorPercent*&quot;</td>
<td>Volume of the reactor contents [%]</td>
<td>&quot;Connections*&quot;</td>
</tr>
</tbody>
</table>
3.5.4. Simulation of the pressure

In the present application example, the pressure simulation is accomplished in the "Pressure" diagram.

The figure below describes the structure of the "Pressure" diagram:

1. Inflow and discharge of inert gas
2. Current gas volume in the reactor
3. Sum of the supplied inert gas
4. Current mass of inert gas in the reactor
5. Calculation of pressure
6. Reactor pressure with uniformly distributed noise of ± 0.001 bar
The following table contains the descriptions for each area:

<table>
<thead>
<tr>
<th>Area</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><strong>Inflow and outflow</strong>&lt;br&gt;Inflow and discharge of the inert gas are calculated as mass flow [kg/h] with the aid of the &quot;Flow&quot; macro. It is assumed that a maximum mass flow rate of 100 kg/h for the inert gas feed and venting is possible. Together, with the current valve position of the inflow or vent valve, the current mass flow is calculated and then converted into kg/s using the &quot;PerHourToPerSecond&quot; macro. The mass flow resulting from the venting is additionally multiplied by &quot;+1&quot;, since the mass is removed from the balance space.</td>
</tr>
<tr>
<td>2</td>
<td><strong>Current gas volume</strong>&lt;br&gt;It is first checked whether the reactor is completely filled with the product. If this is not the case, the current volume of the product in the reactor is used for further calculation. If the reactor is completely filled, a substitute value (reactor volume minus &quot;0.1&quot;) is specified. This is necessary to avoid a division by &quot;0&quot;. The current volume of gas in the reactor is obtained from the difference between the reactor volume and the current volume of the product (or the replacement value) in m³.</td>
</tr>
<tr>
<td>3</td>
<td><strong>Sum of the supplied inert gas</strong>&lt;br&gt;The mass flow of the inert gas is interconnected to an integrator to determine the total amount in kg of inert gas. The time constant of the integrator is 1 second.</td>
</tr>
<tr>
<td>4</td>
<td><strong>Current mass of inert gas</strong>&lt;br&gt;To determine the actual mass of the inert gas, the mass flows of the inflow and venting are added. The sum is then interconnected with an integrator. The time constant of the integrator is 1 second. The result of the integration corresponds to the current mass of inert gas in the reactor in kg.</td>
</tr>
<tr>
<td>5</td>
<td><strong>Maximum mass of the inert gas</strong>&lt;br&gt;The maximum mass of inert gas in the reactor is calculated using the ideal gas law, which is converted according to the mass. The mass of inert gas is the quotient from the product of the maximum pressure in the reactor [Pa] and the reactor volume [m³] and the product of the ideal gas constant for nitrogen and a temperature of 173.15 Kelvin. The calculated value is used in the &quot;pressure&quot; diagram as an integration limit for the integrator.</td>
</tr>
<tr>
<td>6</td>
<td><strong>Calculation of pressure</strong>&lt;br&gt;The pressure in the reactor is calculated using the ideal gas law. The pressure in the reactor corresponds to the quotient from the product of the current mass of gas in the reactor, the gas constant (nitrogen), the current temperature in the reactor and the current volume of gas in the reactor. The air pressure is then added. This gives the pressure in the reactor in Pa. This is converted to bar by multiplying by 1*10⁵.</td>
</tr>
<tr>
<td>7</td>
<td><strong>Reactor pressure with measurement noise</strong>&lt;br&gt;In addition to the calculated reactor pressure in bar, a uniformly distributed measurement noise of ± 0.01 bar is also added. The measurement noise can be switched via an analog value switch and is therefore optional.</td>
</tr>
</tbody>
</table>

### Global connectors

The following table summarizes the global connectors of the "Pressure" diagram, which forwards the values to other diagrams:

<table>
<thead>
<tr>
<th>Connector</th>
<th>Value</th>
<th>Charts</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;SL/SumInertgas&quot;</td>
<td>Total amount of inert gas [kg]</td>
<td>&quot;Connections&quot;</td>
</tr>
<tr>
<td>&quot;SL/PressureReactor&quot;</td>
<td>&quot;Reactor pressure [bar]&quot;</td>
<td>&quot;Connections&quot;</td>
</tr>
</tbody>
</table>
3.5.5. **Simulation of the temperature**

In the present application example, the temperature simulation is accomplished in the "Temp_Jacket" and "Temp_Reactor" diagrams.

"Temp_Jacket"

In the "Temp_Jacket" diagram, the temperature is calculated at the cooling jacket output. The figure below describes the structure of the "Temp_Jacket" diagram:

The diagram is divided into the following 9 areas:

1. Mass flow of the heating medium
2. Temperature of the heating medium
3. Mass flow of the coolant
4. Temperature of the coolant
5. Total heat flow
6. Specific heat capacity of the medium in the cooling jacket
7. Rate of temperature change
8. Temperature of the cooling jacket output
9. Temperature of cooling jacket output with uniformly distributed noise ±1°C
The following table contains the descriptions for each area:

<table>
<thead>
<tr>
<th>Area</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><strong>Mass flow of the heating medium</strong>&lt;br&gt;The mass flow [kg/h] of the heating medium is calculated using the &quot;Flow&quot; macro. It is assumed that a maximum mass flow of 100 kg/h is possible. Together with the current valve position of the control valve for the heating medium, the current mass flow is calculated and then converted into kg/s using the &quot;PerHourToPerSecond&quot; macro.</td>
</tr>
<tr>
<td>2</td>
<td><strong>Temperature of the heating medium</strong>&lt;br&gt;In the temperature simulation of the heating medium, it is assumed that this corresponds to the position of the valve in percent. This means that when the valve is 50% open, the temperature of the heating medium is 50°C. Then the temperature is converted to Kelvin by adding 273.15.</td>
</tr>
<tr>
<td>3</td>
<td><strong>Mass flow of the coolant</strong>&lt;br&gt;The mass flow [kg/h] of the coolant is calculated using the Flow macro. It is assumed that a maximum mass flow of 100 kg/h is possible. In addition to the current valve position of the coolant control valve, the current mass flow is calculated and then converted to kg/s with the PerHourToPerSecond macro.</td>
</tr>
<tr>
<td>4</td>
<td><strong>Temperature of the coolant</strong>&lt;br&gt;In the temperature simulation of the heating medium, it is assumed that this corresponds to the negative position of the valve in percent. This means that when the valve is 50% open, the temperature of the cooling medium is -50°C. Then the temperature is converted to Kelvin by adding 273.15.</td>
</tr>
<tr>
<td>5</td>
<td><strong>Total heat flow</strong>&lt;br&gt;The total heat flow is derived from the sum of the heat flows through the heating medium, the coolant and the heat flow produced by the heat transfer from the reactor to the cooling jacket. The heat flow of the heating medium is calculated using the &quot;Heat_Flow1&quot; macro. The inputs of the macro are interconnected with:&lt;br&gt;• current mass flow of the heating medium [kg/s]&lt;br&gt;• specific heat capacity of the heating medium [m²/s²<em>K]&lt;br&gt;• temperature of the heating medium [K]&lt;br&gt;• temperature of the cooling jacket output [K]&lt;br&gt;The output of the macro is the heat flow of the heating medium in kg</em>m²/s³.&lt;br&gt;The heat flow of the coolant is calculated using the &quot;Heat_Flow1&quot; macro. The inputs of the macro are interconnected with:&lt;br&gt;• current mass flow of the coolant [kg/s]&lt;br&gt;• specific heat capacity of the coolant [m²/s²<em>K]&lt;br&gt;• temperature of the coolant [K]&lt;br&gt;• temperature of the cooling jacket output [K]&lt;br&gt;The output of the macro is the heat flow of the coolant in kg</em>m²/s³.&lt;br&gt;The heat flow resulting from the heat transfer between the reactor and cooling jacket is calculated using the &quot;Heat_Flow2&quot; macro. The inputs of the macro are interconnected with:&lt;br&gt;• heat transfer coefficient [kg/s³<em>K]&lt;br&gt;• heat transfer area [m²]&lt;br&gt;• reactor temperature [K]&lt;br&gt;• mean cooling jacket temperature [K]&lt;br&gt;The output of the macro is the heat flow in kg</em>m²/s³, resulting from the heat transfer between the reactor and cooling jacket.</td>
</tr>
<tr>
<td>6</td>
<td><strong>Specific heat capacity of the medium in the cooling jacket</strong>&lt;br&gt;The medium in the cooling jacket is a mixture of the heating medium and the coolant. It is simply assumed that the specific heat capacity of the medium in the cooling jacket is composed of equal parts of the specific heat capacities of both the heating medium and the coolant.</td>
</tr>
</tbody>
</table>
7  **Rate of temperature change**

The rate of temperature change in the cooling jacket is calculated with the "Rate_of_temperature_change" macro. The inputs of the macro are interconnected with:

- current heat flow \([\text{kg} \cdot \text{m}^2/\text{s}^3]\)
- mass of the medium in the cooling jacket [kg] (assumed to be constant)
- specific heat capacity of the medium in the cooling jacket \([\text{m}^2/\text{s}^2 \cdot \text{K}]\)

The output of the macro is the rate of temperature change in the cooling jacket in K/s.

8  **Temperature of the cooling jacket output**

The current temperature in Kelvin at the cooling jacket outlet is obtained by integrating the rate of temperature change. The time constant of the integrator is 1 second. The upper integration limit is 373.15, the lower integration limit is 173.15. The temperature value in Kelvin is converted to degrees Celsius by subtracting 273.15.

9  **Temperature of the cooling jacket output with measurement noise**

In addition to the calculated temperature of the cooling jacket output in degrees Celsius, a uniformly distributed measurement noise of ± °C is also added. The measurement noise can be switched via an analog value switch and is therefore optional.

**Global connector**

The following table summarizes the global connectors of the "Temp_Jacket" diagram, which forwards the values to other diagrams:

<table>
<thead>
<tr>
<th>Connector</th>
<th>Value</th>
<th>Charts</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;Temp_Heat_Kelvin&quot;</td>
<td>Temperature of the heating medium [K]</td>
<td>&quot;Temp_Reactor&quot;</td>
</tr>
<tr>
<td>&quot;Temp_Cool_Kelvin&quot;</td>
<td>Temperature of the coolant [K]</td>
<td>&quot;Temp_Reactor&quot;</td>
</tr>
<tr>
<td>&quot;SL/TempJacket&quot;</td>
<td>Temperature of the cooling jacket output [°C]</td>
<td>&quot;Connections&quot;</td>
</tr>
</tbody>
</table>
"Temp_Reactor"

In the "Temp_Reactor" diagram, the temperature of the reactor is calculated. The figure below describes the structure of the "Temp_Reactor" diagram:

The diagram is divided into the following 6 areas:
1. Properties of the inflows
2. Total heat flow
3. Rate of temperature change
4. Mean temperature in the cooling jacket
5. Temperature in the reactor
6. Temperature in reactor with uniformly distributed noise ±1°C

The following table contains the descriptions for each area.
### Properties of the inflows

The mass flows of the inflows from the main component, secondary components, and catalyst are converted from kg/h to kg/s using the "PerHourToPerSecond" macro. Temperatures are also converted from degrees Celsius to Kelvin.

### Total heat flow

The total heat flow is derived from the sum of the heat flows through the main component, the secondary component and the heat flow produced by the heat transfer from the reactor to the cooling jacket.

The heat flow of the main component is calculated using the "Heat_Flow1" macro. The inputs of the macro are interconnected with:
- current mass flow of the main component [kg/s]
- specific heat capacity of the main component [m²/s²*K]
- temperature of the main component [K]
- temperature of the reactor [K]

The output of the macro is the heat flow of the main component in kg*m³/s³.

The heat flow of the secondary component 1 is calculated using the "Heat_Flow1" macro. The inputs of the macro are interconnected with:
- current mass flow of the secondary component 1 [kg/s]
- specific heat capacity of the secondary component 1 [m²/s²*K]
- temperature of the secondary component 1 [K]
- temperature of the reactor [K]

The output of the macro is the heat flow of the secondary component 1 in kg*m³/s³.

The heat flow of the secondary component 2 is calculated using the "Heat_Flow1" macro. The inputs of the macro are interconnected with:
- current mass flow of the secondary component 2 [kg/s]
- specific heat capacity of the secondary component 2 [m²/s²*K]
- temperature of the secondary component 2 [K]
- temperature of the reactor [K]

The output of the macro is the heat flow of the secondary component 2 in kg*m³/s³.

The heat flow of the catalyst is calculated using the "Heat_Flow1" macro. The inputs of the macro are interconnected with:
- current mass flow of the catalyst [kg/s]
- specific heat capacity of the catalyst [kg*m²/s³]
- temperature of the catalyst [K]
- temperature of the reactor [K]

The output of the macro is the heat flow of the catalyst in kg*m³/s³.

The heat flow resulting from the heat transfer between the reactor and cooling jacket is calculated using the "Heat_Flow2" macro. The inputs of the macro are interconnected with:
- heat transfer coefficient [kg/s³*K]
- heat transfer area [m²]
- mean temperature of the cooling jacket [K]
- temperature of the reactor [K]

The output of the macro is the heat flow in kg*m³/s³, resulting from the heat transfer between the reactor and cooling jacket.

The heat flows caused by the inflows can be set with analog value switches to a fixed value.

### Rate of temperature change

The rate of temperature change in the cooling jacket is calculated with the "Rate_of_temperature_change" macro. The inputs of the macro are interconnected with:
- current heat flow [kg*m³/s³]
- product weight in the reactor [kg]
- specific heat capacity of the product [m³/s²*K]

The output of the macro is the rate of temperature change in the reactor in K/s.
Mean temperature in the cooling jacket
The mean temperature in the cooling jacket is calculated with the "T_Mean" macro. The inputs of the macro are interconnected with:
- Temperature of the heating medium [K]
- Temperature of the coolant [K]
- Temperature of the cooling jacket output [K]

The macro output is the mean temperature of the cooling jacket.

Temperature in the reactor
The current temperature in Kelvin in the reactor is obtained by integrating the rate of temperature change. The time constant of the integrator is 1 second. The upper integration limit is 373.15, the lower integration limit is 273.15. The temperature value in Kelvin is converted to degrees Celsius by subtracting 273.15.

Temperature of the reactor with measurement noise
In addition to the calculated temperature in the reactor in degrees Celsius, a uniformly distributed measurement noise of ± °C is also added. The measurement noise can be switched via an analog value switch and is therefore optional.

Global connectors
The following table summarizes the global connectors of the "Temp_Reactor" diagram, which forwards the values to other diagrams:

<table>
<thead>
<tr>
<th>Connector</th>
<th>Value</th>
<th>Charts</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;Temp_Mean&quot;</td>
<td>mean temperature of the cooling jacket [K]</td>
<td>&quot;Temp_Jacket&quot;</td>
</tr>
<tr>
<td>&quot;Temp_Reactor&quot;</td>
<td>temperature of the cooling jacket output [K]</td>
<td>&quot;Heat Capacity&quot;  &quot;Pressure&quot;  &quot;Temp_Jacket&quot;</td>
</tr>
<tr>
<td>&quot;SL/TempReactor&quot;</td>
<td>temperature of the cooling jacket output [K]</td>
<td>&quot;Connections&quot;</td>
</tr>
</tbody>
</table>
3.6. Parameters and overview

In the "Physical parameter" plan, all parameters that constitute the basis of calculation of the simulation model are grouped together.

Examples of these are parameters such as density, temperature, heat capacity, and maximum flow of inflowing resources.

If necessary, the parameters in this screen can be adjusted.

For a better overview, the "Reactor overview" plan is included in the project; this shows, at a glance, the most important calculated process values and the operating states of valves and drives. The schematic representation of the reactor shows inflowing media on the left and outflowing resources on the right.
4. Fundamentals – Process Technology

4.1. Process simulation

To simulate a process, an adequate process model must be set up before. Thereby, a compromise between accuracy and generality must be found. The more accurate a process model is built, the better the simulation results. However, an increase in the accuracy of the process model also entails an increase in its complexity. For this reason, a simplified process model is described in this application example.

The individual components of the process model of the stirred tank reactor are described in the following. The entry point is the pipeline and instrument flow diagram (P&I flow diagram).

The figure below shows the P&I flow diagram of the stirred tank reactor:

Assumptions and conditions

The following assumptions/conditions are assumed for the stirred tank reactor shown in the figure:

- The stirred tank reactor possesses any geometry with ideal mixing and jacket cooling.
- Educts and additives are metered separately. In this process, the material flows can have an arbitrary time course.
- The temperature distribution inside of the reactor mixture is considered to be homogeneous.
- The spatial dependence of the coolant temperature (along the coolant flow in the tempering jacket) remains disregarded. The averaged jacket temperature from the input and output temperature is used instead of the temperature gradient in the cooling jacket.
- The heat capacity of the reactor wall (steel) is small when compared to the heat capacity of the reactor mixture and is therefore neglected.
- Heat dissipated from the cooling jacket into the environment is not modeled.
- The heat input from the stirrer or other secondary thermal effects are neglected.

**Physical sizes**

The following table gives an overview of the physical sizes, which are technically detected or known. The units correspond to the measured values and must be still partially converted.

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Formula symbols</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature of the reactor</td>
<td>$T_R$</td>
<td>[°C]</td>
</tr>
<tr>
<td>Temperature of the main component</td>
<td>$T_q$</td>
<td>[°C]</td>
</tr>
<tr>
<td>Temperature of the secondary component 1</td>
<td>$T_{c1}$</td>
<td>[°C]</td>
</tr>
<tr>
<td>Temperature of the secondary component 2</td>
<td>$T_{c2}$</td>
<td>[°C]</td>
</tr>
<tr>
<td>Temperature of the catalyst</td>
<td>$T_{cat}$</td>
<td>[°C]</td>
</tr>
<tr>
<td>Mean jacket temperature</td>
<td>$T_J$</td>
<td>[°C]</td>
</tr>
<tr>
<td>Volume flow of the main component</td>
<td>$\dot{V}_q$</td>
<td>[l/h]</td>
</tr>
<tr>
<td>Volume flow of the secondary component 1</td>
<td>$\dot{V}_{c1}$</td>
<td>[l/h]</td>
</tr>
<tr>
<td>Volume flow of the secondary component 2</td>
<td>$\dot{V}_{c2}$</td>
<td>[l/h]</td>
</tr>
<tr>
<td>Volume flow of the catalyst</td>
<td>$\dot{V}_{cat}$</td>
<td>[l/h]</td>
</tr>
<tr>
<td>Volume flow of the product</td>
<td>$\dot{V}_p$</td>
<td>[l/h]</td>
</tr>
<tr>
<td>Volume flow input of inert gas</td>
<td>$\dot{V}<em>{I</em>{in}}$</td>
<td>$m^3/s$</td>
</tr>
<tr>
<td>Volume flow output of inert gas</td>
<td>$\dot{V}<em>{I</em>{out}}$</td>
<td>$m^3/s$</td>
</tr>
<tr>
<td>Mass flow of the main component</td>
<td>$\dot{m}_q$</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>Mass flow of the secondary component 1</td>
<td>$\dot{m}_{c1}$</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>Mass flow of the secondary component 2</td>
<td>$\dot{m}_{c2}$</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>Mass flow of the catalyst</td>
<td>$\dot{m}_{cat}$</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>Mass flow of the product</td>
<td>$\dot{m}_p$</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>Mass flow of the heating medium</td>
<td>$\dot{m}_{heat}$</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>Mass flow of the coolant</td>
<td>$\dot{m}_{cool}$</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>Mass flow input of inert gas</td>
<td>$\dot{m}<em>{I</em>{in}}$</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>Physical quantity</td>
<td>Formula symbols</td>
<td>Unit</td>
</tr>
<tr>
<td>-----------------------------------------------</td>
<td>-----------------</td>
<td>------------</td>
</tr>
<tr>
<td>Mass flow output of inert gas</td>
<td>( \dot{m}_{\text{fout}} )</td>
<td>([\text{kg/s}])</td>
</tr>
<tr>
<td>Weight of inert gas in the reactor</td>
<td>( m_G )</td>
<td>([\text{kg}])</td>
</tr>
<tr>
<td>Specific heat capacity of the main component</td>
<td>( c_{pq} )</td>
<td>([\text{m}^2/\text{s}^2 \cdot \text{K}])</td>
</tr>
<tr>
<td>Specific heat capacity of the secondary component 1</td>
<td>( c_{pc1} )</td>
<td>([\text{m}^2/\text{s}^2 \cdot \text{K}])</td>
</tr>
<tr>
<td>Specific heat capacity of the secondary component 2</td>
<td>( c_{pc2} )</td>
<td>([\text{m}^2/\text{s}^2 \cdot \text{K}])</td>
</tr>
<tr>
<td>Specific heat capacity of the catalyst</td>
<td>( c_{pcat} )</td>
<td>([\text{m}^2/\text{s}^2 \cdot \text{K}])</td>
</tr>
<tr>
<td>Specific heat capacity of the product</td>
<td>( c_{PP} )</td>
<td>([\text{m}^2/\text{s}^2 \cdot \text{K}])</td>
</tr>
<tr>
<td>Fill level</td>
<td>( h )</td>
<td>([\text{m}])</td>
</tr>
<tr>
<td>Heat flow of the main component</td>
<td>( \dot{Q}_q )</td>
<td>([\text{kg} \cdot \text{m}^2/\text{s}^3])</td>
</tr>
<tr>
<td>Heat flow of the secondary component 1</td>
<td>( \dot{Q}_{c1} )</td>
<td>([\text{kg} \cdot \text{m}^2/\text{s}^3])</td>
</tr>
<tr>
<td>Heat flow of the secondary component 2</td>
<td>( \dot{Q}_{c2} )</td>
<td>([\text{kg} \cdot \text{m}^2/\text{s}^3])</td>
</tr>
<tr>
<td>Heat flow of the catalyst</td>
<td>( \dot{Q}_{cat} )</td>
<td>([\text{kg} \cdot \text{m}^2/\text{s}^3])</td>
</tr>
<tr>
<td>Heat flow of the heating medium</td>
<td>( \dot{Q}_{\text{heat}} )</td>
<td>([\text{kg} \cdot \text{m}^2/\text{s}^3])</td>
</tr>
<tr>
<td>Heat flow of the coolant</td>
<td>( \dot{Q}_{\text{cool}} )</td>
<td>([\text{kg} \cdot \text{m}^2/\text{s}^3])</td>
</tr>
<tr>
<td>Heat transfer between the cooling jacket and reactor</td>
<td>( \dot{Q}_{RJ} )</td>
<td>([\text{kg} \cdot \text{m}^2/\text{s}^3])</td>
</tr>
<tr>
<td>Reactor pressure</td>
<td>( p )</td>
<td>([\text{bar}])</td>
</tr>
<tr>
<td>Reactor volume</td>
<td>( V_R )</td>
<td>([\text{m}^3])</td>
</tr>
<tr>
<td>Gas volume</td>
<td>( V_G )</td>
<td>([\text{m}^3])</td>
</tr>
<tr>
<td>Material volume in the reactor</td>
<td>( V )</td>
<td>([\text{m}^3])</td>
</tr>
<tr>
<td>Reactor floor area</td>
<td>( A_{GR} )</td>
<td>([\text{m}^2])</td>
</tr>
<tr>
<td>Individual gas constant</td>
<td>( R_s )</td>
<td>([\text{m}^2/\text{s}^2 \cdot \text{K}])</td>
</tr>
<tr>
<td>Heat transfer coefficient</td>
<td>( U )</td>
<td>([\text{kg/s}^3 \cdot \text{K}])</td>
</tr>
<tr>
<td>Heat transfer area</td>
<td>( A_{bu} )</td>
<td>([\text{m}^2])</td>
</tr>
</tbody>
</table>

The balance equations can be set up under the above referenced assumptions, based on the known physical sizes and constants.
## 4.2. Mass balance

The mass balance of the reactor can be determined on the basis of inflowing and outflowing masses. The mass flows can be determined with the aid of the volume flows and specific densities of the substances.

The mass flow can be determined using the following formula:

<table>
<thead>
<tr>
<th>Formula</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{m} = \rho \cdot \dot{V}$</td>
<td>( \frac{kg}{s} )</td>
</tr>
</tbody>
</table>

Therefore, the mass balance is the sum of the inflowing and outflowing mass flows:

<table>
<thead>
<tr>
<th>Formula</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{V} = \dot{V}<em>{in} + \dot{V}</em>{out}$</td>
<td>( m^3 )</td>
</tr>
</tbody>
</table>

$\dot{V} = \dot{V}_q + \dot{V}_{c1} + \dot{V}_{c2} + \dot{V}_{cat} + \dot{V}_p$

$\dot{m} = \rho_q \dot{V}_q + \rho_{c1} \dot{V}_{c1} + \rho_{c2} \dot{V}_{c2} + \rho_{cat} \dot{V}_{cat} + \rho_p \dot{V}_p$

$\dot{m} = \dot{m}_q + \dot{m}_{c1} + \dot{m}_{c2} + \dot{m}_{cat} + \dot{m}_p$
4.3. Fill level

The fill level of the reactor can be determined with the aid of the input and output volumes and the geometric properties of reactor (volume, surface area).

The volume and the floor area of the reactor are constants which can be tailored by the user of the application.

In order to calculate the current fill level from the volume flow, the volume change has to be replaced with the following expression:

\[ \dot{V} = A_{GR} \frac{d}{dt} \cdot h(t) \quad \text{[m}^3\text{s}^{-1}] \]

When inserted in the volume flow equation and solved according to the fill level it gives:

\[ A_{GR} \frac{d}{dt} \cdot h(t) = \dot{V}_{in} + \dot{V}_{out} \quad \text{[m}^3\text{s}^{-1}] \]

\[ dh(t) = \frac{1}{A_{GR}} \left( \dot{V}_{in} + \dot{V}_{out} \right) dt \quad \text{[m]} \]

\[ h(t) = \int \frac{1}{A_{GR}} \left( \dot{V}_{in} + \dot{V}_{out} \right) dt \quad \text{[m]} \]
4.4. Heat balance

The stirred tank reactor with cooling jacket is based on two heat balances:

- Heat balance of the stirred tank reactor
- Heat balance of the cooling jacket

The heat balances are conservation equations, which are based on a defined area, the balance space.

**Heat balance reactor**

The balance space of the reactor's interior is used for the heat balance of the reactor. The figure shows the heat flows flowing into and out of the balance space.
The heat balance gives the following as a result:

\[
\frac{dQ_R(t)}{dt} = \dot{Q}_{in} + \dot{Q}_{out}
\]

\[
\frac{dQ_R(t)}{dt} = \dot{Q}_q + \dot{Q}_{c1} + \dot{Q}_{c2} + \dot{Q}_{cat} + \dot{Q}_{RJ}
\]

The change of the stored heat in the reactor is proportional to its temperature change. The proportionality factor here is the general heat capacity \(C_R\) of the reactor mixture, which is composed of the mass and the specific heat capacity of the substance mixture. The following therefore applies:

\[
\frac{dQ_R(t)}{dt} = m_R \cdot c_p \cdot R(t) \cdot \frac{dT_R(t)}{dt}
\]

In each case, the heat supply from the incoming material flows is given from the corresponding mass flow, the specific heat capacity and the temperature difference between the inflow and the reactor contents:

\[
\dot{Q}_q = m_q \cdot c_p \cdot Q \cdot (T_q - T_R)
\]

\[
\dot{Q}_{c1} = m_{c1} \cdot c_{p1} \cdot (T_{c1} - T_R)
\]

\[
\dot{Q}_{c2} = m_{c2} \cdot c_{p2} \cdot (T_{c2} - T_R)
\]

\[
\dot{Q}_{cat} = m_{cat} \cdot c_{pat} \cdot (T_{cat} - T_R)
\]

The heat transfer to the cooling jacket is determined from the heat transfer coefficient \(U\), the heat transfer area \(A\) and the difference between the reactor temperature and the mean cooling jacket temperature:

\[
\dot{Q}_{RJ} = U_{RJ} \cdot A_{RJ} \cdot (T_j - T_R)
\]
In short, one can write the following about the heat balance of the reactor:

\[
\dot{m}_R c_{pr} \frac{dT_R(t)}{dt} = \dot{m}_q c_{pq} (T_q - T_R) + \dot{m}_{c1} c_{pc1} (T_{c1} - T_R) + \dot{m}_{c2} c_{pc2} (T_{c2} - T_R) + \dot{m}_{cat} c_{pcat} (T_{cat} - T_R) + U_R A_R (\bar{T}_J - T_R)
\]

**Heat balance of the cooling jacket**

The cooling jacket itself is taken as a balance space for the heat balance of the cooling jacket.

For the cooling jacket, the figure gives the conservation equation:

\[
\frac{dQ_J(t)}{dt} = \dot{Q}_{in} + \dot{Q}_{out} \\
\frac{dQ_J(t)}{dt} = \dot{Q}_{j,in} + \dot{Q}_{j,out} + \dot{Q}_{Jf}
\]
The change of the stored heat in the cooling jacket is proportional to its temperature change. The proportionality factor here is the general heat capacity of the medium in the cooling jacket, which is composed of the mass and the specific heat capacity of the medium.

The following therefore applies:

<table>
<thead>
<tr>
<th>Formula</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{dQ_j(t)}{dt} = m_j c_p \frac{dT_j(t)}{dt} )</td>
<td>[kg \cdot m^2] [s^3]</td>
</tr>
</tbody>
</table>

In each case, the heat flow from the incoming material flows is given from the corresponding mass flow, the specific heat capacity and the temperature difference between the inflow and the cooling jacket contents:

<table>
<thead>
<tr>
<th>Formula</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{Q}<em>{\text{heat}} = \dot{m}</em>{\text{heat}} c_{\text{heat}} (T_{\text{heat}} - T_j) )</td>
<td>[kg \cdot m^2] [s^3]</td>
</tr>
<tr>
<td>( \dot{Q}<em>{\text{cool}} = \dot{m}</em>{\text{cool}} c_{\text{cool}} (T_{\text{cool}} - T_j) )</td>
<td></td>
</tr>
</tbody>
</table>

The heat transfer between the cooling jacket and the reactor corresponds exactly to the dissipated or supplied heat from the reactor:

<table>
<thead>
<tr>
<th>Formula</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{Q}<em>{B_j} = U</em>{B_j} A_{B_j} (\bar{T}_j - T_R) )</td>
<td>[kg \cdot m^2] [s^3]</td>
</tr>
</tbody>
</table>

In short, one can write the following about the heat balance of the cooling jacket:

<table>
<thead>
<tr>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m_j c_p \frac{dT_j(t)}{dt} = \dot{m}<em>{\text{heat}} c</em>{\text{heat}} (T_{\text{heat}} - T_j) + \dot{m}<em>{\text{cool}} c</em>{\text{cool}} (T_{\text{cool}} - T_j) + U_{B_j} A_{B_j} (\bar{T}_j - T_R) )</td>
</tr>
</tbody>
</table>
4.5. Pressure

In order to calculate the pressure in the reactor, one requires that portion from the total volume of the reactor, which is occupied by the inert gas (e.g. nitrogen). The gas volume is determined from the total reactor volume (constant) and the volume of the reactor contents (variable):

\[ V_G(t) = V_R - V(t) \]  \[ \text{Unit: } m^3 \]

Further, the pressure is dependent on the mass of the inert gas and the temperature in the reactor. The determination of the reactor temperature takes place as described in step 2.4.3. The mass of the inert gas is determined as follows by the incoming and outgoing mass flows:

\[ \frac{dm_G}{dt} = \dot{m}_{\text{in}} + \dot{m}_{\text{out}} \]  \[ \text{Unit: } kg/s \]

\[ m_G(t) = \int (\dot{m}_{\text{in}} + \dot{m}_{\text{out}}) \, dt \]  \[ \text{Unit: } kg \]

The pressure \( p \) can now be determined with the aid of the thermal equation of state for an ideal gas.

\[ p = \frac{m_G R_T}{V_G} \]  \[ \text{Unit: } kg/(m \cdot s^2) \]
5. Appendix

5.1. Service and support

SiePortal
The integrated platform for product selection, purchasing and support - and connection of Industry Mall and Online support. The SiePortal home page replaces the previous home pages of the Industry Mall and the Online Support Portal (SIOS) and combines them.

- Products & Services
  In Products & Services, you can find all our offerings as previously available in Mall Catalog.
- Support
  In Support, you can find all information helpful for resolving technical issues with our products.
- mySiePortal
  mySiePortal collects all your personal data and processes, from your account to current orders, service requests and more. You can only see the full range of functions here after you have logged in.

You can access SiePortal via this address: sieportal.siemens.com

Industry Online Support
Industry Online Support is the previous address for information on our products, solutions and services.

Product information, manuals, downloads, FAQs and application examples - all information is available with just a few mouse clicks: support.industry.siemens.com

Technical Support
The Technical Support of Siemens Industry provides you fast and competent support regarding all technical queries with numerous tailor-made offers – ranging from basic support to individual support contracts.

Please send queries to Technical Support via Web form: support.industry.siemens.com/cs/my/src

SITRAIN – Digital Industry Academy
We support you with our globally available training courses for industry with practical experience, innovative learning methods and a concept that's tailored to the customer's specific needs.

For more information on our offered trainings and courses, as well as their locations and dates, refer to our web page: siemens.com/sitrain

Industry Online Support app
You will receive optimum support wherever you are with the "Industry Online Support" app. The app is available for iOS and Android:
5.2. Links and literature

<table>
<thead>
<tr>
<th>Nr.</th>
<th>Thema</th>
</tr>
</thead>
</table>
| 1.1 | Siemens Industry Online Support  
https://support.industry.siemens.com |
| 1.2 | Link to this entry page of this application example  
| 1.3 | |

5.3. Change documentation

<table>
<thead>
<tr>
<th>Version</th>
<th>Date</th>
<th>Modification</th>
</tr>
</thead>
<tbody>
<tr>
<td>V1.0</td>
<td>06/2014</td>
<td>First edition</td>
</tr>
<tr>
<td>V2.0</td>
<td>01/2021</td>
<td>Revision and adaptation to current versions</td>
</tr>
<tr>
<td>V3.0</td>
<td>08/2022</td>
<td>Revision and adaptation to current versions</td>
</tr>
<tr>
<td>V4.0</td>
<td>08/2023</td>
<td>Revision and adaptation to current versions</td>
</tr>
</tbody>
</table>