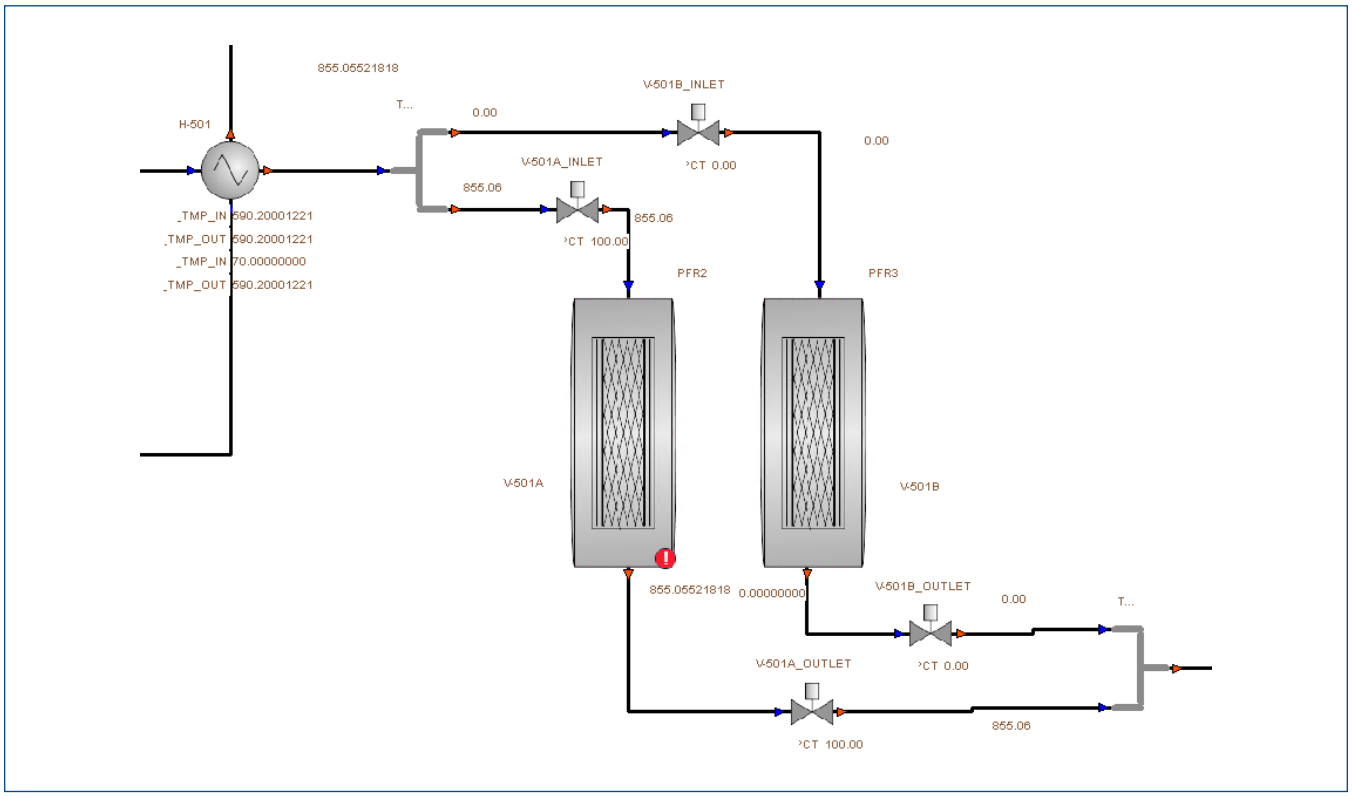
# Mimic™ Process – Reactions




- Intuitive unit operation modeling
- Supports wide variety of process reactors
- Calculates dynamic material and energy balances, and Vapor Liquid Equilibrium
- Provides built-in guides for Reactions and Kinetics Configurations

## Introduction

Mimic™ Reactions Process Objects provide high fidelity dynamic models of chemical reactors designed for high-performance simulations for operator training or automation system testing.

The Mimic Process – Reactions Package is an add-on to the Mimic Process – Separations package that includes sophisticated process objects into the Mimic Simulation Studio modeling palette. These objects can be used on Mimic systems for application software testing, operator training, and process or operation improvements.

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## Benefits

**Intuitive unit operation modeling**

These process objects come with modeling infrastructure that makes the development of accurate models quick and easy.

**Supports wide variety of process reactors**

The reactor operation can be continuous, batch, semi-batch, or any combination of these modes. Continuous Stirred Tank Reactors and Plug Flow Reactors are both supported.

**Calculates dynamic material, energy, and VLE balances**

The reactor model calculates the dynamic material, energy, and VLE balances resulting from the reaction mixture interaction with external streams, chemical transformations due to the reaction kinetics, and interaction with ambient conditions. The energy balance includes also the heat exchange with the reactor's jacket or internal coil and optional agitator.

**Provides built-in guides for Reactions and Kinetics Configurations**

Included guides offer knowledge and instructions on how to define reaction types and reaction orders and evaluate the reaction parameters from the available data.

## Product Description

The Mimic Process – Reactions package provides high-fidelity dynamic models for unit operations commonly found in chemical processing plants as well as other industries with industrial reactions.

Each process object in the Mimic Reactions Process Package includes specific parameters designed for quick configuration.

**Continuous Stirred Tank Reactor**

The Continuous Stirred Tank Reactor Process Object provides a high-fidelity dynamic model with several features that makes it suitable for simulation of a wide variety of the industrial reactors.

This object can handle main kinetic reaction types such as General Kinetic 1, General Kinetic 2, Heterogeneous Catalytic Reaction Kinetics. The reaction can occur in the gas, liquid, or overall (mixed gas/liquid) phase. The Reaction Phase is specified for each of the reactions of the given reaction system. The Reaction object can handle up to 20 simultaneous reactions as forward, reverse or equilibrium equations.

The reaction can be specified as Active or Inactive. The Active reaction participates in the kinetic calculations; the Inactive is ignored at the run time calculations, i.e. its rate is automatically assigned to zero.

Configuration of the Continuous Stirred Tank Reactor includes:

- Up to 8 input feeds, plus an optional stream for the heat exchanging jacket or internal coil.
- Up to 8 output draws, plus an optional outlet stream for the heat exchanging jacket or internal coil.
- Reactions based on the chosen component sets. The main component set defines what materials are in the reactor, while the 2nd component set defines the reactions occurring in the reactor.
- Agitation definition to link the controller based, physical equipment elements to the reaction kinetics as defined in the reaction dynamics of each reaction.
- Examination of the components in the set, providing a list of independent reactions from the list of materials and a stoichiometric breakdown of the reactions.

**Plug Flow Reactor**

The Plug Flow Reactor Process Object provides a high-fidelity dynamic model with features that make it suitable for reactor designs that consist of continuous vessels, pipes or tubes and possess a thermal and concentration gradient with respect to length. Mimic subdivides the volume of the reactor into a series of sections, and each section is assumed to have lumped behavior. This object assumes no holdup which mean that all mass entering the object will be present in the outflow of the same time step. However, the composition and temperature will be changed according to the reactions taking place.

The Plug Flow Reactor allows the configuration of two sides of material, i.e. Process Fluid and Media Fluid. The Process Fluid enters the reactor and undergoes the configured reaction. The Media Fluid is optional. It undergoes heat exchange with the process fluid according to user specification. User defined Number_Of_Sections determine how many volumes the PFR uses within its execution. As the number of sections increases, the better the modeling follows the expected behavior of a PFR.

This object can handle main kinetic reaction types such as General Kinetic 1, General Kinetic 2, Heterogeneous Catalytic Reaction Kinectics. The reaction can occur in the gas, liquid, or overall (mixed gas/liquid) phase. The Reaction Phase is specified for each of the reactions of the given reaction system. The Reaction object can handle up to 20 simultaneous reactions as forward, reverse or equilibrium equations.

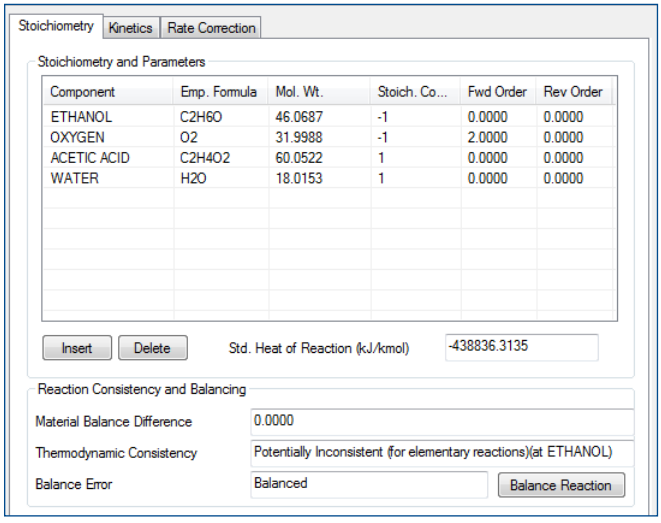
Configuration of the Plug Flow Reactor includes:

- Catalyst and reactor mass heat transfer effects.
- Reactions based on the chosen component sets.
  The main component set defines what materials are in the reactor, while the 2nd component set defines the reactions occurring in the reactor.
- Examination of the components in the set, providing a list of independent reactions from the list of materials and a stoichiometric breakdown of the reactions.

### Configuration Reaction Assistant

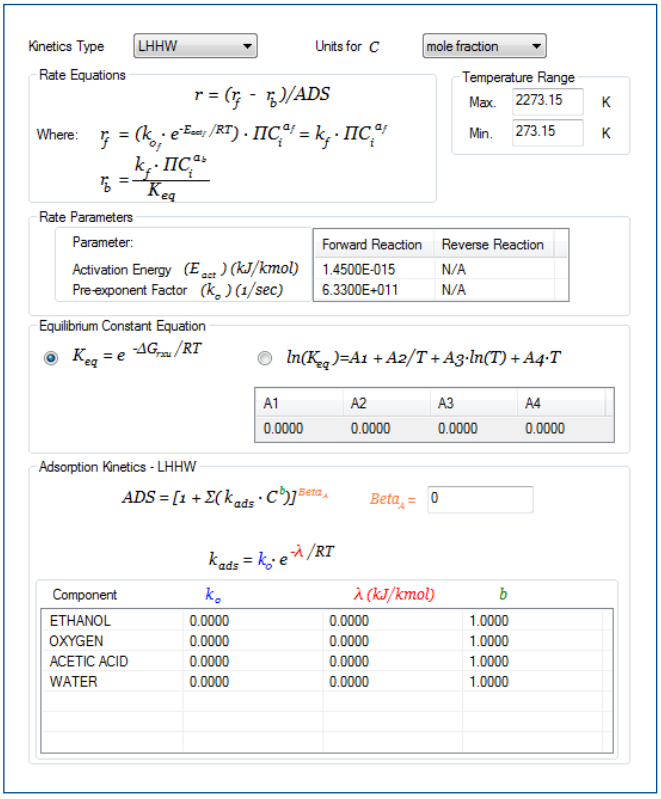
The Configuration Reaction Assistant guides you through the creation of the Reaction Set that will be used by the object. The Reaction Set, containing all necessary data on the reactions that occur in the reaction system (at the gas, liquid and/or combine phases of the reactor), is created by step by step procedure in the Configuration Assistant or can be imported from the Library of the Predefined Reaction sets.

The run time functionality of the Kinetic Reactor object includes dynamic calculation of the material and heat balances resulting from the reaction mixture interaction with external streams (material and heat ones), chemical transformations according to the reaction kinetics, and due to vapor liquid equilibrium (VLE). The energy balance includes also the heat exchange with Jacket/Coil, ambient conditions, and heat input from Agitator (if applicable).




### Kinetic Reaction Assistant

The Kinetic Reaction Assistant, consisting of the Reaction Kinetics Guide and Reaction Kinetics Tutorial, provides a guided approach to developing a model of the chemical kinetics and primary analysis of kinetic data from the laboratory and industrial reactors.




The Kinetics Guide provides knowledge and instructions on how to define the reaction type, reaction order, and evaluate the reaction parameters from the available experimental data. It provides a more detailed insight into the reaction kinetics, including the reactor types, general models for each type of the reactors, and basic definitions and relations of the chemical kinetics.

### Reactor View

The run time Reactor Views provides real-time trends and profiles of the main reactor variables, providing a deep insight into the object performance. The set of strip charts contains views for: inlet/outlet flow rates of the vessel, pressure/temperature and vapor fraction in the reactor, vapor and liquid holdup and composition changes, reaction rate constants and reaction rates, net rate of change of the components, and the reactor jacket and agitator performance (if applicable).

## Ordering Information

The Mimic Process – Reactions license can be added to any Mimic system by first adding both the Mimic Process – Core and Separations licenses.

| Description | Model Number |
|---|---|
| Mimic Process – Core | MM3-7111 |
| Mimic Process – Separations | MM3-7121 |
| Mimic Process – Reactions | MM3-7141 |



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