

Rate-Controlled Reactions

To add kinetic type reactions to your Powerlaw Reaction ID:

- 1 Click New on the Reactions Stoichiometry sheet of your Powerlaw Reaction ID.
- 2 On the Edit Reaction dialog box, Reaction Type defaults to Kinetic, and the reaction number is entered automatically. Enter components and stoichiometric coefficients to define the reaction. Coefficients should be negative for reactants and positive for products.
- 3 Specify power law exponents for the components. These exponents represent the *order* of the reaction with respect to each component. If you do not specify an exponent for a component, Aspen Plus uses a default value of 0.
- 4 Click Close when finished. You should see your new reaction number, type, and equation displayed on the Stoichiometry sheet.
- 5 Repeat steps 1 through 4 for each additional kinetic reaction.
- 6 Select the Kinetic sheet.
- 7 On the Kinetic sheet, select a reaction from the list at the top of the sheet.
- 8 Specify in which phase the reaction will take place in the Reacting Phase field. The default is the liquid phase.
- 9 Enter the pre-exponential factor (k), the temperature exponent (n), and the activation energy (E) in the appropriate fields. The pre-exponential factor must be in the SI units described later in this section. The temperature exponent refers to temperature in Kelvin.
- 10 In the [Ci] Basis list, select the concentration basis. The concentration basis determines which form of the power law expression will be used, as discussed later in this section.
- 11 If solids are present, click the Solids button and select the appropriate options for calculation of concentration. For more information, see [Reactions With Solids](#).
- 12 Repeat steps 7 through 11 for each kinetic reaction.

The power law expression depends on the concentration basis you select in the [Ci] Basis list:

[Ci] Basis	<u>Power Law Expression</u> (To is not specified)	<u>Power Law Expression</u> (To is specified)
Molarity (default)	$r = kT^n e^{-E/RT} \prod (C_i)^{\alpha_i}$	$r = k(T/T_o)^n e^{(-E/R)[1/T-1/T_o]} \prod (C_i)^{\alpha_i}$
Molality (electrolytes only)	$r = kT^n e^{-E/RT} \prod (m_i)^{\alpha_i}$	$r = k(T/T_o)^n e^{(-E/R)[1/T-1/T_o]} \prod (m_i)^{\alpha_i}$
Mole fraction	$r = kT^n e^{-E/RT} \prod (x_i)^{\alpha_i}$	$r = k(T/T_o)^n e^{(-E/R)[1/T-1/T_o]} \prod (x_i)^{\alpha_i}$
Mass fraction	$r = kT^n e^{-E/RT} \prod (x_i^m)^{\alpha_i}$	$r = k(T/T_o)^n e^{(-E/R)[1/T-1/T_o]} \prod (x_i^m)^{\alpha_i}$
Partial pressure (vapor only)	$r = kT^n e^{-E/RT} \prod (p_i)^{\alpha_i}$	$r = k(T/T_o)^n e^{(-E/R)[1/T-1/T_o]} \prod (p_i)^{\alpha_i}$
Mass concentration	$r = kT^n e^{-E/RT} \prod (C_i^m)^{\alpha_i}$	$r = k(T/T_o)^n e^{(-E/R)[1/T-1/T_o]} \prod (C_i^m)^{\alpha_i}$

The units of the reaction rate and the pre-exponential factor depend on the:

- Order of the reaction
- Concentration basis selected in the [Ci] Basis list box

The units for the pre-exponential factor are as follows:

When [Ci] Basis is	Units are: (To is not specified)	Units are: (To is specified)
Molarity	$\frac{\text{kgmole} \cdot \text{K}^{-n}}{\text{sec} - \text{m}^3}$ $\left(\frac{\text{kgmole}}{\text{m}^3} \right)^{\sum \alpha_i}$	$\frac{\text{kgmole}}{\text{sec} - \text{m}^3}$ $\left(\frac{\text{kgmole}}{\text{m}^3} \right)^{\sum \alpha_i}$
Molality	$\frac{\text{kgmole} \cdot \text{K}^{-n}}{\text{sec} - \text{m}^3}$ $\left(\frac{\text{gmole}}{\text{kg H}_2\text{O}} \right)^{\sum \alpha_i}$	$\frac{\text{kgmole}}{\text{sec} - \text{m}^3}$ $\left(\frac{\text{gmole}}{\text{kg H}_2\text{O}} \right)^{\sum \alpha_i}$
Mole fraction or Mass fraction	$\frac{\text{kgmole} \cdot \text{K}^{-n}}{\text{sec} - \text{m}^3}$	$\frac{\text{kgmole}}{\text{sec} - \text{m}^3}$
Partial pressure	$\frac{\text{kgmole} \cdot \text{K}^{-n}}{\text{sec} - \text{m}^3}$ $\left(\frac{\text{N}}{\text{m}^2} \right)^{\sum \alpha_i}$	$\frac{\text{kgmole}}{\text{sec} - \text{m}^3}$ $\left(\frac{\text{N}}{\text{m}^2} \right)^{\sum \alpha_i}$
Mass concentration	$\frac{\text{kgmole} \cdot \text{K}^{-n}}{\text{sec} - \text{m}^3}$ $\left(\frac{\text{kg}}{\text{m}^3} \right)^{\sum \alpha_i}$	$\frac{\text{kgmole}}{\text{sec} - \text{m}^3}$ $\left(\frac{\text{kg}}{\text{m}^3} \right)^{\sum \alpha_i}$

