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Basics of Reactor Design and Temperature Dependency from Arrhenius Law Formulas

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Basics of Reactor Design and Temperature Dependency from Arrhenius Law C

1) Activation Energy using Rate Constant at Two Different Temperatures

fx
$$\mathbf{E}_{\mathrm{a2}} = [\mathrm{R}] \cdot \ln\!\left(rac{\mathrm{K}_2}{\mathrm{K}_1}
ight) \cdot \mathrm{T}_1 \cdot rac{\mathrm{T}_2}{\mathrm{T}_2 - \mathrm{T}_1}$$

$$220.736 \text{J/mol} = [\text{R}] \cdot \ln\left(\frac{26.2/\text{s}}{21/\text{s}}\right) \cdot 30\text{K} \cdot \frac{40\text{K}}{40\text{K} - 30\text{K}}$$

2) Activation Energy using Reaction Rate at Two Different Temperatures 🖸

fx
$$\mathbf{E}_{a1} = [\mathrm{R}] \cdot \ln \left(rac{\mathrm{r}_2}{\mathrm{r}_1}
ight) \cdot \mathrm{T}_1 \cdot rac{\mathrm{T}_2}{\mathrm{T}_2 - \mathrm{T}_1}$$

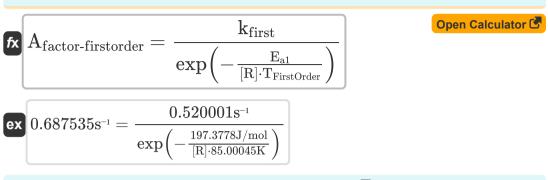
$$\text{ex} \ 197.3778 \text{J/mol} = [\text{R}] \cdot \ln \left(\frac{19.5 \text{mol/m}^{3} \text{*s}}{16 \text{mol/m}^{3} \text{*s}} \right) \cdot 30 \text{K} \cdot \frac{40 \text{K}}{40 \text{K} - 30 \text{K}}$$



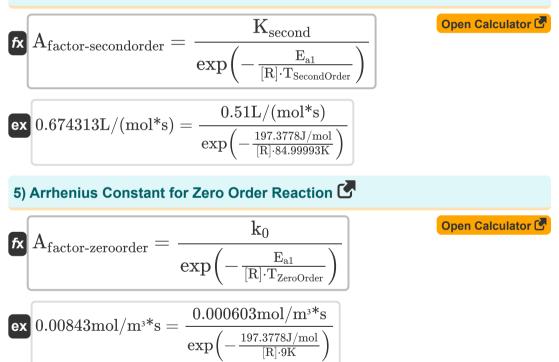
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3) Arrhenius Constant for First Order Reaction



4) Arrhenius Constant for Second Order Reaction 🕑





6) Initial Key Reactant Concentration with Varying Density, Temperature and Total Pressure

fx
$$\mathbf{C}_{\mathrm{key0}} = \mathbf{C}_{\mathrm{key}} \cdot \left(\frac{1 + \epsilon \cdot \mathbf{X}_{\mathrm{key}}}{1 - \mathbf{X}_{\mathrm{key}}} \right) \cdot \left(\frac{\mathbf{T}_{\mathrm{CRE}} \cdot \pi_0}{\mathbf{T}_0 \cdot \pi} \right)$$

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$$\boxed{13.03566 \text{mol}/\text{m}^{3} = 34 \text{mol}/\text{m}^{3} \cdot \left(\frac{1 + 0.21 \cdot 0.3}{1 - 0.3}\right) \cdot \left(\frac{85 \text{K} \cdot 45 \text{Pa}}{303 \text{K} \cdot 50 \text{Pa}}\right)}$$

7) Initial Reactant Concentration using Reactant Conversion 🕑

fx
$$m C_o=rac{C}{1-X_A}$$
ex $m 80mol/m^3=rac{24mol/m^3}{1-0.7}$

8) Initial Reactant Concentration using Reactant Conversion with Varying Density

fx
$$Intial_{Conc} = rac{(C) \cdot (1 + \epsilon \cdot X_A)}{1 - X_A}$$

ex $91.76 mol/m^3 = rac{(24 mol/m^3) \cdot (1 + 0.21 \cdot 0.7)}{1 - 0.7}$



9) Initial Reactant Conversion using Reactant Concentration with Varying Density

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ex
$$0.658514 = rac{80 \mathrm{mol}/\mathrm{m^3} - 24 \mathrm{mol}/\mathrm{m^3}}{80 \mathrm{mol}/\mathrm{m^3} + 0.21 \cdot 24 \mathrm{mol}/\mathrm{m^3}}$$

 $\mathbf{X}_{\mathrm{A}} = rac{\mathrm{C}_{0} - \mathrm{C}}{\mathrm{C}_{0} + \epsilon \cdot \mathrm{C}}$

10) Key Reactant Concentration with Varying Density, Temperature and Total Pressure

fx
$$\mathbf{C}_{\mathrm{key}} = \mathbf{C}_{\mathrm{key0}} \cdot \left(\frac{1 - \mathbf{X}_{\mathrm{key}}}{1 + \epsilon \cdot \mathbf{X}_{\mathrm{key}}} \right) \cdot \left(\frac{\mathbf{T}_0 \cdot \pi}{\mathbf{T}_{\mathrm{CRE}} \cdot \pi_0} \right)$$

Open Calculator 🕑

$$34.00001 \mathrm{mol/m^{3}} = 13.03566 \mathrm{mol/m^{3}} \cdot \left(rac{1-0.3}{1+0.21\cdot0.3}
ight) \cdot \left(rac{303 \mathrm{K} \cdot 50 \mathrm{Pa}}{85 \mathrm{K} \cdot 45 \mathrm{Pa}}
ight)$$

11) Key Reactant Conversion with Varying Density, Temperature and Total Pressure

$$\mathbf{fx} \mathbf{X}_{key} = \frac{1 - \left(\left(\frac{C_{key}}{C_{key0}} \right) \cdot \left(\frac{T_{CRE} \cdot \pi_0}{T_0 \cdot \pi} \right) \right)}{1 + \epsilon \cdot \left(\left(\frac{C_{key}}{C_{key0}} \right) \cdot \left(\frac{T_{CRE} \cdot \pi_0}{T_0 \cdot \pi} \right) \right)}$$
$$\mathbf{ex} \mathbf{0.3} = \frac{1 - \left(\left(\frac{34 \text{mol/m}^3}{13.03566 \text{mol/m}^3} \right) \cdot \left(\frac{85 \text{K} \cdot 45 \text{Pa}}{303 \text{K} \cdot 50 \text{Pa}} \right) \right)}{1 + 0.21 \cdot \left(\left(\frac{34 \text{mol/m}^3}{13.03566 \text{mol/m}^3} \right) \cdot \left(\frac{85 \text{K} \cdot 45 \text{Pa}}{303 \text{K} \cdot 50 \text{Pa}} \right) \right)}$$

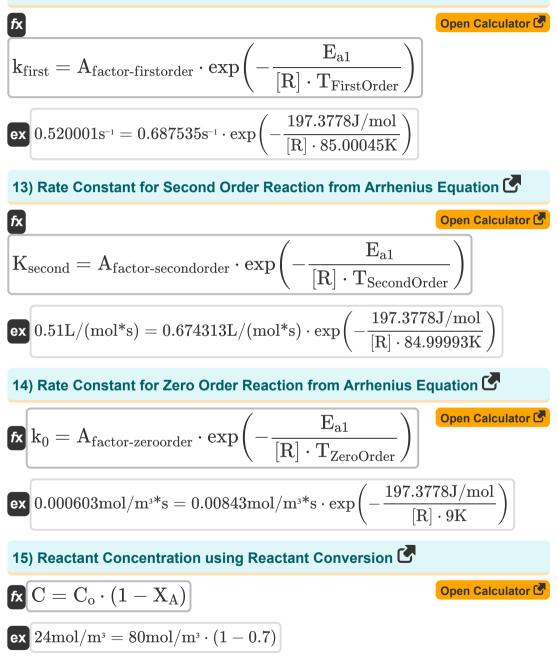




ex

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12) Rate Constant for First Order Reaction from Arrhenius Equation





16) Reactant Concentration using Reactant Conversion with Varying Density

fx
$$\mathrm{C}_{\mathrm{VD}} = rac{(1 - \mathrm{XA}_{\mathrm{VD}}) \cdot (\mathrm{C}_0)}{1 + \epsilon \cdot \mathrm{XA}_{\mathrm{VD}}}$$

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Open Calculator

ex
$$13.69863 ext{mol}/ ext{m}^{3} = rac{(1 - 0.8) \cdot (80 ext{mol}/ ext{m}^{3})}{1 + 0.21 \cdot 0.8}$$

17) Reactant Conversion using Reactant Concentration

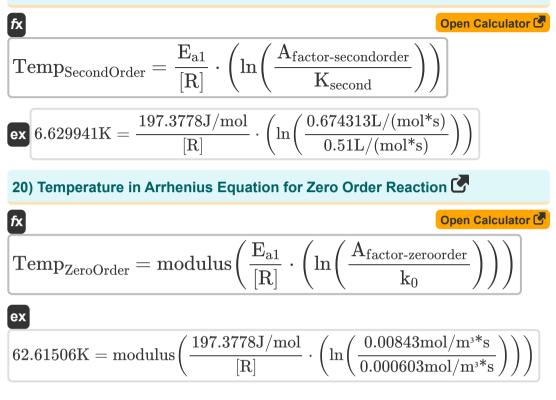
fx
$$X_{
m A}=1-\left(rac{
m C}{
m C_o}
ight)$$
 ex $0.7=1-\left(rac{
m 24mol/m^3}{
m 80mol/m^3}
ight)$

18) Temperature in Arrhenius Equation for First Order Reaction

$$\begin{aligned} & \underbrace{\text{Open Calculator } \ensuremath{\mathbb{C}}}_{\text{Temp}_{FirstOrder}} = modulus \bigg(\frac{E_{a1}}{[R]} \cdot \bigg(\ln \bigg(\frac{A_{factor-firstorder}}{k_{first}} \bigg) \bigg) \bigg) \end{aligned}$$



19) Temperature in Arrhenius Equation for Second Order Reaction





Variables Used

- Afactor-firstorder Frequency Factor from Arrhenius Eqn for 1st Order (1 Per Second)
- Afactor-secondorder Frequency Factor from Arrhenius Eqn for 2nd Order (*Liter per Mole Second*)
- Afactor-zeroorder Frequency Factor from Arrhenius Eqn for Zero Order (Mole per Cubic Meter Second)
- C Reactant Concentration (Mole per Cubic Meter)
- C₀ Initial Reactant Concentration (Mole per Cubic Meter)
- Ckey Key-Reactant Concentration (Mole per Cubic Meter)
- Ckev0 Initial Key-Reactant Concentration (Mole per Cubic Meter)
- **C**_o Initial Reactant Concentration (Mole per Cubic Meter)
- C_{VD} Reactant Concentration with Varying Density (Mole per Cubic Meter)
- Ea1 Activation Energy (Joule Per Mole)
- Ea2 Activation Energy Rate Constant (Joule Per Mole)
- Intial_{Conc} Initial Reactant Conc with Varying Density (Mole per Cubic Meter)
- k₀ Rate Constant for Zero Order Reaction (Mole per Cubic Meter Second)
- K₁ Rate Constant at Temperature 1 (1 Per Second)
- K₂ Rate Constant at Temperature 2 (1 Per Second)
- k_{first} Rate Constant for First Order Reaction (1 Per Second)
- Ksecond Rate Constant for Second Order Reaction (Liter per Mole Second)
- **r**₁ Reaction Rate 1 (Mole per Cubic Meter Second)
- **r**₂ Reaction Rate 2 (Mole per Cubic Meter Second)



- **T**₀ Initial Temperature (*Kelvin*)
- **T₁** Reaction 1 Temperature (*Kelvin*)
- **T₂** Reaction 2 Temperature (Kelvin)
- T_{CRE} Temperature (Kelvin)
- **T**_{FirstOrder} Temperature for First Order Reaction (Kelvin)
- **T**SecondOrder Temperature for Second Order Reaction (Kelvin)
- TzeroOrder Temperature for Zero Order Reaction (Kelvin)
- **Temp_{FirstOrder}** Temperature in Arrhenius Eq for 1st Order Reaction (*Kelvin*)
- Temp_{SecondOrder} Temperature in Arrhenius Eq for 2nd Order Reaction (Kelvin)
- TempzeroOrder Temperature in Arrhenius Eq Zero Order Reaction (Kelvin)
- X_A Reactant Conversion
- Xkev Key-Reactant Conversion
- XAVD Reactant Conversion with Varying Density
- ε Fractional Volume Change
- **π** Total Pressure (Pascal)
- **π₀** Initial Total Pressure (*Pascal*)



Constants, Functions, Measurements used

- Constant: **[R]**, 8.31446261815324 Joule / Kelvin * Mole Universal gas constant
- Function: **exp**, exp(Number) Exponential function
- Function: In, In(Number) Natural logarithm function (base e)
- Function: modulus, modulus Modulus of number
- Measurement: Temperature in Kelvin (K) Temperature Unit Conversion
- Measurement: Pressure in Pascal (Pa) Pressure Unit Conversion
- Measurement: Molar Concentration in Mole per Cubic Meter (mol/m³)
 Molar Concentration Unit Conversion
- Measurement: Energy Per Mole in Joule Per Mole (J/mol) Energy Per Mole Unit Conversion
- Measurement: Reaction Rate in Mole per Cubic Meter Second (mol/m^{3*}s) *Reaction Rate Unit Conversion*
- Measurement: First Order Reaction Rate Constant in 1 Per Second (s⁻¹) First Order Reaction Rate Constant Unit Conversion
- Measurement: Second Order Reaction Rate Constant in Liter per Mole Second (L/(mol*s))
 Second Order Reaction Rate Constant Unit Conversion
- Measurement: Time Inverse in 1 Per Second (1/s)
 Time Inverse Unit Conversion



Check other formula lists

- Basics of Chemical Reaction
 Engineering Formulas
- Basics of Parallel & Single Reactions Formulas
- Basics of Reactor Design and Temperature Dependency from Arrhenius Law Formulas
- Forms of Reaction Rate
 Formulas
- Important Formulas in Basics of Chemical Reaction Engineering & Forms of Reaction Rate
- Important Formulas in Constant and Variable Volume Batch Reactor

- Important Formulas in Constant Volume Batch Reactor for First, Second & Third Order Reaction
- Important Formulas in Design of Reactors & Recycle Reactors for Single Reactions
- Important Formulas in Potpourri of Multiple Reactions
- Reactor Performance Equations for Constant Volume Reactions Formulas
- Reactor Performance Equations for Variable Volume Reactions Formulas

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