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Basics of Reactor Design and Temperature Dependency from Arrhenius Law Formulas

Calculators!

Examples!

Conversions!

List of 20 Basics of Reactor Design and Temperature Dependency from Arrhenius Law Formulas

Basics of Reactor Design and Temperature Dependency from Arrhenius Law

1) Activation Energy using Rate Constant at Two Different Temperatures

Open Calculator

fx $$E_{a2} = [R] \cdot \ln\left(\frac{K_2}{K_1}\right) \cdot T_1 \cdot \frac{T_2}{T_2 - T_1}$$

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

2) Activation Energy using Reaction Rate at Two Different Temperatures

Open Calculator

fx $$E_{a1} = [R] \cdot \ln\left(\frac{r_2}{r_1}\right) \cdot T_1 \cdot \frac{T_2}{T_2 - T_1}$$

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

3) Arrhenius Constant for First Order Reaction

Open Calculator

fx $$A_{\text{factor-firstorder}} = \frac{k_{\text{first}}}{\exp\left(-\frac{E_{a1}}{[R] \cdot T_{\text{FirstOrder}}}\right)}$$

ex $$0.687535\text{s}^{-1} = \frac{0.520001\text{s}^{-1}}{\exp\left(-\frac{197.3778\text{J/mol}}{[R] \cdot 85.00045\text{K}}\right)}$$

4) Arrhenius Constant for Second Order Reaction

Open Calculator

fx $$A_{\text{factor-secondorder}} = \frac{K_{\text{second}}}{\exp\left(-\frac{E_{a1}}{[R] \cdot T_{\text{SecondOrder}}}\right)}$$

ex $$0.674313\text{L/(mol*s)} = \frac{0.51\text{L/(mol*s)}}{\exp\left(-\frac{197.3778\text{J/mol}}{[R] \cdot 84.99993\text{K}}\right)}$$

5) Arrhenius Constant for Zero Order Reaction

Open Calculator

fx $$A_{\text{factor-zeroorder}} = \frac{k_0}{\exp\left(-\frac{E_{a1}}{[R] \cdot T_{\text{ZeroOrder}}}\right)}$$

ex $$0.00843\text{mol/m}^3\text{*s} = \frac{0.000603\text{mol/m}^3\text{*s}}{\exp\left(-\frac{197.3778\text{J/mol}}{[R] \cdot 9\text{K}}\right)}$$

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

Open Calculator

fx $$C_{key0} = C_{key} \cdot \left(\frac{1 + \varepsilon \cdot X_{key}}{1 - X_{key}} \right) \cdot \left(\frac{T_{CRE} \cdot \pi_0}{T_0 \cdot \pi} \right)$$

ex $$13.03566 \text{mol/m³} = 34 \text{mol/m³} \cdot \left(\frac{1 + 0.21 \cdot 0.3}{1 - 0.3} \right) \cdot \left(\frac{85\text{K} \cdot 45\text{Pa}}{303\text{K} \cdot 50\text{Pa}} \right)$$

7) Initial Reactant Concentration using Reactant Conversion

Open Calculator

fx $$C_o = \frac{C}{1 - X_A}$$

ex $$80 \text{mol/m³} = \frac{24 \text{mol/m³}}{1 - 0.7}$$

8) Initial Reactant Concentration using Reactant Conversion with Varying Density

Open Calculator

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

ex $$91.76 \text{mol/m³} = \frac{(24 \text{mol/m³}) \cdot (1 + 0.21 \cdot 0.7)}{1 - 0.7}$$

9) Initial Reactant Conversion using Reactant Concentration with Varying Density

Open Calculator

fx $$X_A = \frac{C_0 - C}{C_0 + \varepsilon \cdot C}$$

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

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

Open Calculator

fx $$C_{key} = C_{key0} \cdot \left(\frac{1 - X_{key}}{1 + \varepsilon \cdot X_{key}} \right) \cdot \left(\frac{T_0 \cdot \pi}{T_{CRE} \cdot \pi_0} \right)$$

ex $$34.00001\text{mol/m}^3 = 13.03566\text{mol/m}^3 \cdot \left(\frac{1 - 0.3}{1 + 0.21 \cdot 0.3} \right) \cdot \left(\frac{303\text{K} \cdot 50\text{Pa}}{85\text{K} \cdot 45\text{Pa}} \right)$$

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

Open Calculator

fx $$X_{key} = \frac{1 - \left(\left(\frac{C_{key}}{C_{key0}} \right) \cdot \left(\frac{T_{CRE} \cdot \pi_0}{T_0 \cdot \pi} \right) \right)}{1 + \varepsilon \cdot \left(\left(\frac{C_{key}}{C_{key0}} \right) \cdot \left(\frac{T_{CRE} \cdot \pi_0}{T_0 \cdot \pi} \right) \right)}$$

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

12) Rate Constant for First Order Reaction from Arrhenius Equation

Open Calculator

fx
$$k_{\text{first}} = A_{\text{factor-firstorder}} \cdot \exp\left(-\frac{E_{a1}}{[R] \cdot T_{\text{FirstOrder}}}\right)$$

ex
$$0.520001\text{s}^{-1} = 0.687535\text{s}^{-1} \cdot \exp\left(-\frac{197.3778\text{J/mol}}{[R] \cdot 85.00045\text{K}}\right)$$

13) Rate Constant for Second Order Reaction from Arrhenius Equation

Open Calculator

fx
$$K_{\text{second}} = A_{\text{factor-secondorder}} \cdot \exp\left(-\frac{E_{a1}}{[R] \cdot T_{\text{SecondOrder}}}\right)$$

ex
$$0.51\text{L/(mol*s)} = 0.674313\text{L/(mol*s)} \cdot \exp\left(-\frac{197.3778\text{J/mol}}{[R] \cdot 84.99993\text{K}}\right)$$

14) Rate Constant for Zero Order Reaction from Arrhenius Equation

Open Calculator

fx
$$k_0 = A_{\text{factor-zeroorder}} \cdot \exp\left(-\frac{E_{a1}}{[R] \cdot T_{\text{ZeroOrder}}}\right)$$

ex
$$0.000603\text{mol/m}^3\text{*s} = 0.00843\text{mol/m}^3\text{*s} \cdot \exp\left(-\frac{197.3778\text{J/mol}}{[R] \cdot 9\text{K}}\right)$$

15) Reactant Concentration using Reactant Conversion

Open Calculator

fx
$$C = C_o \cdot (1 - X_A)$$

ex
$$24\text{mol/m}^3 = 80\text{mol/m}^3 \cdot (1 - 0.7)$$

16) Reactant Concentration using Reactant Conversion with Varying Density

Open Calculator

$$C_{VD} = \frac{(1 - XA_{VD}) \cdot (C_0)}{1 + \varepsilon \cdot XA_{VD}}$$

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

17) Reactant Conversion using Reactant Concentration

Open Calculator

$$X_A = 1 - \left(\frac{C}{C_o}\right)$$

$$0.7 = 1 - \left(\frac{24\text{mol/m}^3}{80\text{mol/m}^3}\right)$$

18) Temperature in Arrhenius Equation for First Order Reaction

Open Calculator

$$\text{Temp}_{\text{FirstOrder}} = \text{modulus}\left(\frac{E_{a1}}{[R]} \cdot \left(\ln\left(\frac{A_{\text{factor-firstorder}}}{k_{\text{first}}}\right)\right)\right)$$

$$6.629901\text{K} = \text{modulus}\left(\frac{197.3778\text{J/mol}}{[R]} \cdot \left(\ln\left(\frac{0.687535\text{s}^{-1}}{0.520001\text{s}^{-1}}\right)\right)\right)$$

19) Temperature in Arrhenius Equation for Second Order Reaction

fx Open Calculator

$$\text{Temp}_{\text{SecondOrder}} = \frac{E_{a1}}{[R]} \cdot \left(\ln\left(\frac{A_{\text{factor-secondorder}}}{K_{\text{second}}} \right) \right)$$

ex

$$6.629941\text{K} = \frac{197.3778\text{J/mol}}{[R]} \cdot \left(\ln\left(\frac{0.674313\text{L/(mol*s)}}{0.51\text{L/(mol*s)}} \right) \right)$$

20) Temperature in Arrhenius Equation for Zero Order Reaction

fx Open Calculator

$$\text{Temp}_{\text{ZeroOrder}} = \text{modulus}\left(\frac{E_{a1}}{[R]} \cdot \left(\ln\left(\frac{A_{\text{factor-zeroorder}}}{k_0} \right) \right) \right)$$

ex

$$62.61506\text{K} = \text{modulus}\left(\frac{197.3778\text{J/mol}}{[R]} \cdot \left(\ln\left(\frac{0.00843\text{mol/m}^3\text{*s}}{0.000603\text{mol/m}^3\text{*s}} \right) \right) \right)$$

Variables Used

- $A_{factor-firstorder}$ Frequency Factor from Arrhenius Eqn for 1st Order *(1 Per Second)*
- $A_{factor-secondorder}$ Frequency Factor from Arrhenius Eqn for 2nd Order *(Liter per Mole Second)*
- $A_{factor-zeroorder}$ Frequency Factor from Arrhenius Eqn for Zero Order *(Mole per Cubic Meter Second)*
- C Reactant Concentration *(Mole per Cubic Meter)*
- C_0 Initial Reactant Concentration *(Mole per Cubic Meter)*
- C_{key} Key-Reactant Concentration *(Mole per Cubic Meter)*
- C_{key0} 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)*
- E_{a1} Activation Energy *(Joule Per Mole)*
- E_{a2} Activation Energy Rate Constant *(Joule Per Mole)*
- $Intial_{Conc}$ Initial Reactant Conc with Varying Density *(Mole per Cubic Meter)*
- k_0 Rate Constant for Zero Order Reaction *(Mole per Cubic Meter Second)*
- K_1 Rate Constant at Temperature 1 *(1 Per Second)*
- K_2 Rate Constant at Temperature 2 *(1 Per Second)*
- k_{first} Rate Constant for First Order Reaction *(1 Per Second)*
- K_{second} 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)*
- T_1 Reaction 1 Temperature *(Kelvin)*
- T_2 Reaction 2 Temperature *(Kelvin)*
- T_{CRE} Temperature *(Kelvin)*
- $T_{FirstOrder}$ Temperature for First Order Reaction *(Kelvin)*
- $T_{SecondOrder}$ Temperature for Second Order Reaction *(Kelvin)*
- $T_{ZeroOrder}$ 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)*
- $Temp_{ZeroOrder}$ Temperature in Arrhenius Eq Zero Order Reaction *(Kelvin)*
- X_A Reactant Conversion
- X_{key} Key-Reactant Conversion
- XA_{VD} Reactant Conversion with Varying Density
- ε Fractional Volume Change
- π Total Pressure *(Pascal)*
- π_0 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: **ln**, ln(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/m³*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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