Important Basics of Reactor Design and Temperature Dependency from Arrhenius Law Formulas PDF

Formulas
Examples
with Units

List of 20

Important Basics of Reactor Design and Temperature Dependency from Arrhenius Law Formulas

1) Activation Energy using Rate Constant at Two Different Temperatures Formula

Evaluate Formula

Formula

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

Example with Units

$$220.736\,\mathrm{J/mol} = 8.3145 \cdot \ln\left(\frac{26.2\,\mathrm{1/s}}{21\,\mathrm{1/s}}\right) \cdot 30\,\mathrm{K} \cdot \frac{40\,\mathrm{K}}{40\,\mathrm{K} - 30\,\mathrm{K}}$$

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

Evaluate Formula

Formula

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

Example with Units

$$197.3778\,\mathrm{J/mol} = 8.3145 \cdot \ln\left(\frac{19.5\,\mathrm{mol/m^3*s}}{16\,\mathrm{mol/m^3*s}}\right) \cdot 30\,\mathrm{K} \cdot \frac{40\,\mathrm{K}}{40\,\mathrm{K} - 30\,\mathrm{K}}$$

3) Arrhenius Constant for First Order Reaction Formula

Evaluate Formula

Formula

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

Example with Units

$$0.6875\,\mathrm{s^{-1}} = \frac{0.520001\,\mathrm{s^{-1}}}{\exp\left(-\frac{197.3778\,\mathrm{J/mol}}{8.3145 \cdot 85.00045\,\mathrm{K}}\right)}$$

4) Arrhenius Constant for Second Order Reaction Formula

Evaluate Formula

Formula

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

Example with Units

$$0.6743\,\text{L/(mol*s)} = \frac{0.51\,\text{L/(mol*s)}}{\exp\left(-\frac{197.3778\,\text{J/mol}}{8.3145 \cdot 84.99993\,\text{K}}\right)}$$

5) Arrhenius Constant for Zero Order Reaction Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0084\,\text{mol/m}^3\text{*s} = \frac{0.000603\,\text{mol/m}^3\text{*s}}{\exp\left(-\frac{197.3778\,\text{J/mol}}{8.3145 \cdot 9\,\text{K}}\right)}$$

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

Evaluate Formula

Formula

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

Example with Units

$$13.0357\,\text{mol/m}^3 = 34\,\text{mol/m}^3 \cdot \left(\frac{1 + 0.21 \cdot 0.3}{1 - 0.3}\right) \cdot \left(\frac{85\,\text{K} \cdot 45\,\text{Pa}}{303\,\text{K} \cdot 50\,\text{Pa}}\right)$$

7) Initial Reactant Concentration using Reactant Conversion Formula

Evaluate Formula

Formula

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

Example with Units

$$80\,\text{mol/m}^3 = \frac{24\,\text{mol/m}^3}{1 - 0.7}$$

8) Initial Reactant Concentration using Reactant Conversion with Varying Density Formula

Evaluate Formula

Formula

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

Example with Units

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

9) Initial Reactant Conversion using Reactant Concentration with Varying Density Formula

Evaluate Formula

Formula

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

Example with Units

$$0.6585 = \frac{80\,\text{mol/m}^3 - 24\,\text{mol/m}^3}{80\,\text{mol/m}^3 + 0.21 \cdot 24\,\text{mol/m}^3}$$

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

Evaluate Formula

Formula

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

Example with Units

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

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

Evaluate Formula

Formula

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

Example with Units

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

12) Rate Constant for First Order Reaction from Arrhenius Equation Formula

Evaluate Formula

Formula

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

Example with Units

$$0.52\,\text{s}^{-1} = 0.687535\,\text{s}^{-1} \cdot \exp\left(- \frac{197.3778\,\text{J/mol}}{8.3145 \cdot 85.00045\,\text{K}} \right)$$

13) Rate Constant for Second Order Reaction from Arrhenius Equation Formula

Evaluate Formula

Formula

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

Example with Units

$$0.51\,\mathrm{L/(mol*s)} = 0.674313\,\mathrm{L/(mol*s)} \cdot \exp\left(-\frac{197.3778\,\mathrm{J/mol}}{8.3145 \cdot 84.99993\,\mathrm{K}} \right)$$

14) Rate Constant for Zero Order Reaction from Arrhenius Equation Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0006\,\mathrm{mol/m^3{*}s} = 0.00843\,\mathrm{mol/m^3{*}s} \cdot \exp\left(-\frac{197.3778\,\mathrm{J/mol}}{8.3145 \cdot 9\,\mathrm{K}} \right)$$

15) Reactant Concentration using Reactant Conversion Formula

Evaluate Formula

Formula

$$C = C_o \cdot \left(1 - X_A \right)$$

Example with Units

$$24\,\mathrm{mol/m^3} = 80\,\mathrm{mol/m^3} \cdot \left(1 - 0.7 \right)$$

16) Reactant Concentration using Reactant Conversion with Varying Density Formula

Evaluate Formula

Formula

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

Example with Units

$$13.6986\,\mathrm{mol/m^3} = \frac{\left(1 - 0.8 \right) \cdot \left(80\,\mathrm{mol/m^3} \right)}{1 + 0.21 \cdot 0.8}$$

17) Reactant Conversion using Reactant Concentration Formula

Evaluate Formula

Formula

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

Example with Units

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

18) Temperature in Arrhenius Equation for First Order Reaction Formula

Evaluate Formula

Formula

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

Example with Units

$$6.6299\,\text{K} = \text{mod}\,us\left(\frac{197.3778\,\text{J/mol}}{8.3145} \cdot \left(\ln\left(\frac{0.687535\,\text{s}^{-1}}{0.520001\,\text{s}^{-1}}\right)\right)\right)$$

19) Temperature in Arrhenius Equation for Second Order Reaction Formula

Evaluate Formula

Formula

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

Example with Units

$$6.6299\,\text{K} = \frac{197.3778\,\text{J/mol}}{8.3145} \cdot \left(\ln\left(\frac{0.674313\,\text{L/(mol*s)}}{0.51\,\text{L/(mol*s)}}\right)\right)$$

20) Temperature in Arrhenius Equation for Zero Order Reaction Formula

Evaluate Formula

Formula

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

Example with Units

$$62.6151\,\text{K} = \text{mod}\,us\left(\frac{197.3778\,\text{J/mol}}{8.3145} \cdot \left(\ln\left(\frac{0.00843\,\text{mol/m}^3\text{*s}}{0.000603\,\text{mol/m}^3\text{*s}}\right)\right)\right)$$

Variables used in list of Basics of Reactor Design and Temperature Dependency from Arrhenius Law Formulas above

- $A_{factor-firstorder}$ 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_{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)*

Constants, Functions, Measurements used in list of Basics of Reactor Design and Temperature Dependency from Arrhenius Law Formulas above

- constant(s): **[R]**, 8.31446261815324
  Universal gas constant
- Functions: **exp**, exp(Number)
  n an exponential function, the value of the function changes by a constant factor for every unit change in the independent variable.
- Functions: **ln**, ln(Number)
  The natural logarithm, also known as the logarithm to the base e, is the inverse function of the natural exponential function.
- Functions: **modulus**, modulus
  Modulus of a number is the remainder when that number is divided by another 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

- 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)*

7/9/2024 | 1:49:54 PM UTC