

Important Basics of Potpourri Reactions Formulas PDF



Formulas Examples with Units

List of 16 Important Basics of Potpourri Reactions Formulas

1) Initial Reactant Concentration for First Order Rxn for MFR using Intermediate Concentration Formula ↻

Formula

Evaluate Formula ↻

$$C_{A0} = \frac{C_R \cdot \left(1 + \left(k_I \cdot \tau_m\right)\right) \cdot \left(1 + \left(k_2 \cdot \tau_m\right)\right)}{k_I \cdot \tau_m}$$

Example with Units

$$23.4889 \text{ mol/m}^3 = \frac{10 \text{ mol/m}^3 \cdot \left(1 + \left(0.42 \text{ s}^{-1} \cdot 12 \text{ s}\right)\right) \cdot \left(1 + \left(0.08 \text{ s}^{-1} \cdot 12 \text{ s}\right)\right)}{0.42 \text{ s}^{-1} \cdot 12 \text{ s}}$$

2) Initial Reactant Concentration for First Order Rxn in MFR at Maximum Intermediate Concentration Formula ↻

Formula

Evaluate Formula ↻

$$C_{A0} = C_{R,\max} \cdot \left(\left(\left(\left(\frac{k_2}{k_I} \right)^{\frac{1}{2}} \right) + 1 \right)^2 \right)$$

Example with Units

$$82.5339 \text{ mol/m}^3 = 40 \text{ mol/m}^3 \cdot \left(\left(\left(\left(\frac{0.08 \text{ s}^{-1}}{0.42 \text{ s}^{-1}} \right)^{\frac{1}{2}} \right) + 1 \right)^2 \right)$$

3) Initial Reactant Concentration for First Order Rxn in Series for Maximum Intermediate Concentration Formula ↻

Formula

Example with Units

Evaluate Formula ↻

$$C_{A0} = \frac{C_{R,\max}}{\left(\frac{k_I}{k_2} \right)^{\frac{k_2}{k_2 - k_I}}}$$

$$59.0894 \text{ mol/m}^3 = \frac{40 \text{ mol/m}^3}{\left(\frac{0.42 \text{ s}^{-1}}{0.08 \text{ s}^{-1}} \right)^{\frac{0.08 \text{ s}^{-1}}{0.08 \text{ s}^{-1} - 0.42 \text{ s}^{-1}}}}$$



4) Initial Reactant Concentration for First Order Rxn in Series for MFR using Product Concentration Formula

Formula

Evaluate Formula 

$$C_{A0} = \frac{C_S \cdot \left(1 + (k_1 \cdot \tau_m)\right) \cdot \left(1 + (k_2 \cdot \tau_m)\right)}{k_1 \cdot k_2 \cdot \left(\tau_m^2\right)}$$

Example with Units

$$48.9352 \text{ mol/m}^3 = \frac{20 \text{ mol/m}^3 \cdot \left(1 + (0.42 \text{ s}^{-1} \cdot 12 \text{ s})\right) \cdot \left(1 + (0.08 \text{ s}^{-1} \cdot 12 \text{ s})\right)}{0.42 \text{ s}^{-1} \cdot 0.08 \text{ s}^{-1} \cdot \left(12 \text{ s}^2\right)}$$

5) Initial Reactant Concentration for Two Steps First Order Irreversible Reaction in Series Formula

Formula

Evaluate Formula 

$$C_{A0} = \frac{C_R \cdot (k_2 - k_1)}{k_1 \cdot \left(\exp(-k_1 \cdot \tau) - \exp(-k_2 \cdot \tau)\right)}$$

Example with Units

$$89.2386 \text{ mol/m}^3 = \frac{10 \text{ mol/m}^3 \cdot (0.08 \text{ s}^{-1} - 0.42 \text{ s}^{-1})}{0.42 \text{ s}^{-1} \cdot \left(\exp(-0.42 \text{ s}^{-1} \cdot 30 \text{ s}) - \exp(-0.08 \text{ s}^{-1} \cdot 30 \text{ s})\right)}$$

6) Initial Reactant Concentration for Two Steps First Order Reaction for Mixed Flow Reactor Formula

Formula

Example with Units

Evaluate Formula 

$$C_{A0} = C_{k1} \cdot \left(1 + (k_1 \cdot \tau_m)\right)$$

$$80.332 \text{ mol/m}^3 = 13.3 \text{ mol/m}^3 \cdot \left(1 + (0.42 \text{ s}^{-1} \cdot 12 \text{ s})\right)$$

7) Intermediate Concentration for First Order Reaction for Mixed Flow Reactor Formula

Formula

Evaluate Formula 

$$C_R = \frac{C_{A0} \cdot k_1 \cdot \tau_m}{\left(1 + (k_1 \cdot \tau_m)\right) \cdot \left(1 + (k_2 \cdot \tau_m)\right)}$$

Example with Units

$$34.0587 \text{ mol/m}^3 = \frac{80 \text{ mol/m}^3 \cdot 0.42 \text{ s}^{-1} \cdot 12 \text{ s}}{\left(1 + (0.42 \text{ s}^{-1} \cdot 12 \text{ s})\right) \cdot \left(1 + (0.08 \text{ s}^{-1} \cdot 12 \text{ s})\right)}$$



8) Intermediate Concentration for Two Steps First Order Irreversible Reaction in Series

Formula

Evaluate Formula 

$$C_R = C_{A0} \cdot \left(\frac{k_1}{k_2 - k_1} \right) \cdot \left(\exp(-k_1 \cdot \tau) - \exp(-k_2 \cdot \tau) \right)$$

Example with Units

$$8.9647 \text{ mol/m}^3 = 80 \text{ mol/m}^3 \cdot \left(\frac{0.42 \text{ s}^{-1}}{0.08 \text{ s}^{-1} - 0.42 \text{ s}^{-1}} \right) \cdot \left(\exp(-0.42 \text{ s}^{-1} \cdot 30 \text{ s}) - \exp(-0.08 \text{ s}^{-1} \cdot 30 \text{ s}) \right)$$

9) Maximum Intermediate Concentration for First Order Irreversible Reaction in MFR

Formula

Evaluate Formula 

Formula

$$C_{R,\max} = \frac{C_{A0}}{\left(\left(\left(\frac{k_2}{k_1} \right)^{\frac{1}{2}} + 1 \right)^2 \right)}$$

Example with Units

$$38.7719 \text{ mol/m}^3 = \frac{80 \text{ mol/m}^3}{\left(\left(\left(\frac{0.08 \text{ s}^{-1}}{0.42 \text{ s}^{-1}} \right)^{\frac{1}{2}} + 1 \right)^2 \right)}$$

10) Maximum Intermediate Concentration for First Order Irreversible Reaction in Series

Formula

Evaluate Formula 

Formula

$$C_{R,\max} = C_{A0} \cdot \left(\frac{k_1}{k_2} \right)^{\frac{k_2}{k_2 - k_1}}$$

Example with Units

$$54.1553 \text{ mol/m}^3 = 80 \text{ mol/m}^3 \cdot \left(\frac{0.42 \text{ s}^{-1}}{0.08 \text{ s}^{-1}} \right)^{\frac{0.08 \text{ s}^{-1}}{0.08 \text{ s}^{-1} - 0.42 \text{ s}^{-1}}}$$

11) Product Concentration for First Order Reaction for Mixed Flow Reactor

Formula

Evaluate Formula 

Formula

$$C_S = \frac{C_{A0} \cdot k_1 \cdot k_2 \cdot (\tau_m^2)}{(1 + (k_1 \cdot \tau_m)) \cdot (1 + (k_2 \cdot \tau_m))}$$

Example with Units

$$32.6963 \text{ mol/m}^3 = \frac{80 \text{ mol/m}^3 \cdot 0.42 \text{ s}^{-1} \cdot 0.08 \text{ s}^{-1} \cdot (12 \text{ s})^2}{(1 + (0.42 \text{ s}^{-1} \cdot 12 \text{ s})) \cdot (1 + (0.08 \text{ s}^{-1} \cdot 12 \text{ s}))}$$

12) Rate Constant for First Step First Order Reaction for MFR at Maximum Intermediate Concentration

Formula

Evaluate Formula 

Formula

$$k_1 = \frac{1}{k_2 \cdot (\tau_{R,\max}^2)}$$

Example with Units

$$0.2785 \text{ s}^{-1} = \frac{1}{0.08 \text{ s}^{-1} \cdot (6.7 \text{ s})^2}$$



13) Rate Constant for Second Step First Order Reaction for MFR at Maximum Intermediate Concentration Formula

Formula

$$k_2 = \frac{1}{k_1 \cdot (\tau_{R,\max})^2}$$

Example with Units

$$0.053 \text{ s}^{-1} = \frac{1}{0.42 \text{ s}^{-1} \cdot (6.7 \text{ s})^2}$$

Evaluate Formula 

14) Reactant Concentration for Two Steps First Order Reaction for Mixed Flow Reactor Formula

Formula

$$C_{k0} = \frac{C_{A0}}{1 + (k_1 \cdot \tau_m)}$$

Example with Units

$$13.245 \text{ mol/m}^3 = \frac{80 \text{ mol/m}^3}{1 + (0.42 \text{ s}^{-1} \cdot 12 \text{ s})}$$

Evaluate Formula 

15) Time at Maximum Intermediate Concentration for First Order Irreversible Reaction in Series Formula

Formula

$$\tau_{R,\max} = \frac{\ln\left(\frac{k_2}{k_1}\right)}{k_2 - k_1}$$

Example with Units

$$4.8771 \text{ s} = \frac{\ln\left(\frac{0.08 \text{ s}^{-1}}{0.42 \text{ s}^{-1}}\right)}{0.08 \text{ s}^{-1} - 0.42 \text{ s}^{-1}}$$

Evaluate Formula 

16) Time at Maximum Intermediate Concentration for First Order Irreversible Reaction in Series in MFR Formula

Formula

$$\tau_{R,\max} = \frac{1}{\sqrt{k_1 \cdot k_2}}$$

Example with Units

$$5.4554 \text{ s} = \frac{1}{\sqrt{0.42 \text{ s}^{-1} \cdot 0.08 \text{ s}^{-1}}}$$

Evaluate Formula 



Variables used in list of Basics of Potpourri Reactions Formulas above

- **C_{A0}** Initial Reactant Concentration for Multiple Rxns (Mole per Cubic Meter)
- **C_{k0}** Reactant Concentration for Zero Order Series Rxn (Mole per Cubic Meter)
- **C_{k1}** Reactant Concentration for 1st Order Series Rxns (Mole per Cubic Meter)
- **C_R** Intermediate Concentration for Series Rxn (Mole per Cubic Meter)
- **$C_{R,max}$** Maximum Intermediate Concentration (Mole per Cubic Meter)
- **C_S** Final Product Concentration (Mole per Cubic Meter)
- **k_2** Rate Constant for Second Step First Order Reaction (1 Per Second)
- **k_1** Rate Constant for First Step First Order Reaction (1 Per Second)
- **T** Space Time for PFR (Second)
- **T_m** Space Time for Mixed Flow Reactor (Second)
- **$T_{R,max}$** Time at Maximum Intermediate Concentration (Second)

Constants, Functions, Measurements used in list of Basics of Potpourri Reactions Formulas above

- **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: sqrt**, sqrt(Number)
A square root function is a function that takes a non-negative number as an input and returns the square root of the given input number.
- **Measurement: Time** in Second (s)
Time Unit Conversion 
- **Measurement: Molar Concentration** in Mole per Cubic Meter (mol/m³)
Molar Concentration Unit Conversion 
- **Measurement: First Order Reaction Rate Constant** in 1 Per Second (s⁻¹)
First Order Reaction Rate Constant Unit Conversion 



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