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Basics of Potpourri Reactions Formulas

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List of 16 Basics of Potpourri Reactions Formulas

Basics of Potpourri Reactions

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

Open Calculator

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

ex $$23.48889\text{mol/m}^3 = \frac{10\text{mol/m}^3 \cdot (1 + (0.42\text{s}^{-1} \cdot 12\text{s})) \cdot (1 + (0.08\text{s}^{-1} \cdot 12\text{s}))}{0.42\text{s}^{-1} \cdot 12\text{s}}$$

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

Open Calculator

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

ex $$82.53391\text{mol/m}^3 = 40\text{mol/m}^3 \cdot \left(\left(\left(\left(\frac{0.08\text{s}^{-1}}{0.42\text{s}^{-1}}\right)^{\frac{1}{2}}\right) + 1\right)^2\right)$$

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

Open Calculator

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

ex $$59.08935\text{mol/m}^3 = \frac{40\text{mol/m}^3}{\left(\frac{0.42\text{s}^{-1}}{0.08\text{s}^{-1}}\right)^{\frac{0.08\text{s}^{-1}}{0.08\text{s}^{-1} - 0.42\text{s}^{-1}}}}$$

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

Open Calculator

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

ex $$48.93519\text{mol/m}^3 = \frac{20\text{mol/m}^3 \cdot (1 + (0.42\text{s}^{-1} \cdot 12\text{s})) \cdot (1 + (0.08\text{s}^{-1} \cdot 12\text{s}))}{0.42\text{s}^{-1} \cdot 0.08\text{s}^{-1} \cdot \left((12\text{s})^2\right)}$$

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

Open Calculator

fx $$C_{A0} = \frac{C_R \cdot (k_2 - k_I)}{k_I \cdot (\exp(-k_I \cdot \tau) - \exp(-k_2 \cdot \tau))}$$

ex $$89.23855\text{mol/m}^3 = \frac{10\text{mol/m}^3 \cdot (0.08\text{s}^{-1} - 0.42\text{s}^{-1})}{0.42\text{s}^{-1} \cdot (\exp(-0.42\text{s}^{-1} \cdot 30\text{s}) - \exp(-0.08\text{s}^{-1} \cdot 30\text{s}))}$$

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

Open Calculator

fx $$C_{A0} = C_{k1} \cdot (1 + (k_I \cdot \tau_m))$$

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

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

Open Calculator

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

ex $$34.05866\text{mol/m}^3 = \frac{80\text{mol/m}^3 \cdot 0.42\text{s}^{-1} \cdot 12\text{s}}{(1 + (0.42\text{s}^{-1} \cdot 12\text{s})) \cdot (1 + (0.08\text{s}^{-1} \cdot 12\text{s}))}$$

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

Open Calculator

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

ex $$8.964735\text{mol/m}^3 = 80\text{mol/m}^3 \cdot \left(\frac{0.42\text{s}^{-1}}{0.08\text{s}^{-1} - 0.42\text{s}^{-1}}\right) \cdot (\exp(-0.42\text{s}^{-1} \cdot 30\text{s}) - \exp(-0.08\text{s}^{-1} \cdot 30\text{s}))$$

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

Open Calculator

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

ex $$38.77194\text{mol/m}^3 = \frac{80\text{mol/m}^3}{\left(\left(\left(\frac{0.08\text{s}^{-1}}{0.42\text{s}^{-1}}\right)^{\frac{1}{2}}\right)+1\right)^2}$$

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

Open Calculator

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

ex $$54.15527\text{mol/m}^3 = 80\text{mol/m}^3\cdot\left(\frac{0.42\text{s}^{-1}}{0.08\text{s}^{-1}}\right)^{\frac{0.08\text{s}^{-1}}{0.08\text{s}^{-1}-0.42\text{s}^{-1}}}$$

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

Open Calculator

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

ex $$32.69631\text{mol/m}^3 = \frac{80\text{mol/m}^3\cdot 0.42\text{s}^{-1}\cdot 0.08\text{s}^{-1}\cdot\left((12\text{s})^2\right)}{(1+(0.42\text{s}^{-1}\cdot 12\text{s}))\cdot(1+(0.08\text{s}^{-1}\cdot 12\text{s}))}$$

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

Open Calculator

fx $$k_I = \frac{1}{k_2\cdot\left(\tau_{R,max}^2\right)}$$

ex $$0.278458\text{s}^{-1} = \frac{1}{0.08\text{s}^{-1}\cdot\left((6.7\text{s})^2\right)}$$

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

Open Calculator

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

$$0.05304\text{s}^{-1} = \frac{1}{0.42\text{s}^{-1} \cdot \left((6.7\text{s})^2\right)}$$

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

Open Calculator

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

$$13.24503\text{mol/m}^3 = \frac{80\text{mol/m}^3}{1 + (0.42\text{s}^{-1} \cdot 12\text{s})}$$

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

Open Calculator

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

$$4.877141\text{s} = \frac{\ln\left(\frac{0.08\text{s}^{-1}}{0.42\text{s}^{-1}}\right)}{0.08\text{s}^{-1} - 0.42\text{s}^{-1}}$$

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

Open Calculator

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

$$5.455447\text{s} = \frac{1}{\sqrt{0.42\text{s}^{-1} \cdot 0.08\text{s}^{-1}}}$$

Variables Used

- 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)*
- τ Space Time for PFR *(Second)*
- τ_m Space Time for Mixed Flow Reactor *(Second)*
- $\tau_{R,max}$ Time at Maximum Intermediate Concentration *(Second)*

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Constants, Functions, Measurements used

- Function: **exp**, exp(Number)
  Exponential function
- Function: **ln**, ln(Number)
  Natural logarithm function (base e)
- Function: **sqrt**, sqrt(Number)
  Square root function
- 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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- **Basics of Potpourri Reactions Formulas**
- **Zero Order followed by First Order Reaction Formulas**

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