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Important Formulas in Potpourri of Multiple Reactions

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List of 26 Important Formulas in Potpourri of Multiple Reactions

Important Formulas in Potpourri of Multiple 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 $$59.08935\text{mol/m}^3 = \frac{40\text{mol/m}^3}{\left(\frac{0.42\text{s}^{-1}}{0.08\text{s}^{-1}} \right)^{\frac{0.08\text{s}^{-1}}{0.08\text{s}^{-1} - 0.42\text{s}^{-1}}}}$$

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) Initial Reactant Concentration in First Order followed by Zero Order Reaction

Open Calculator

fx $$C_{A0} = \frac{C_{k0}}{\exp(-k_I \cdot \Delta t)}$$

ex $$84.61012\text{mol/m}^3 = \frac{24\text{mol/m}^3}{\exp(-0.42\text{s}^{-1} \cdot 3\text{s})}$$

8) Initial Reactant Concentration using Intermediate for First Order followed by Zero Order Reaction

Open Calculator

fx $$C_{A0\text{ for R}} = \frac{C_R + (k_0 \cdot \Delta t)}{1 - \exp(-k_I \cdot \Delta t)}$$

ex $$41.18122\text{mol/m}^3 = \frac{10\text{mol/m}^3 + (6.5\text{mol/m}^3\text{*s} \cdot 3\text{s})}{1 - \exp(-0.42\text{s}^{-1} \cdot 3\text{s})}$$

9) Intermediate Concentration for First Order followed by Zero Order Reaction

Open Calculator

fx $$C_{R,1st\ order} = C_{A0} \cdot \left(1 - \exp(-k_I \cdot \Delta t) - \left(\frac{k_0 \cdot \Delta t}{C_{A0}}\right)\right)$$

ex $$37.80768\text{mol/m}^3 = 80\text{mol/m}^3 \cdot \left(1 - \exp(-0.42\text{s}^{-1} \cdot 3\text{s}) - \left(\frac{6.5\text{mol/m}^3\text{*s} \cdot 3\text{s}}{80\text{mol/m}^3}\right)\right)$$

10) 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 $$34.05866\text{mol/m}^3 = \frac{80\text{mol/m}^3 \cdot 0.42\text{s}^{-1} \cdot 12\text{s}}{(1 + (0.42\text{s}^{-1} \cdot 12\text{s})) \cdot (1 + (0.08\text{s}^{-1} \cdot 12\text{s}))}$$

11) 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 $$8.964735\text{mol/m}^3 = 80\text{mol/m}^3 \cdot \left(\frac{0.42\text{s}^{-1}}{0.08\text{s}^{-1} - 0.42\text{s}^{-1}}\right) \cdot (\exp(-0.42\text{s}^{-1} \cdot 30\text{s}) - \exp(-0.08\text{s}^{-1} \cdot 30\text{s}))$$

12) 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 $$38.77194\text{mol/m}^3 = \frac{80\text{mol/m}^3}{\left(\left(\left(\frac{0.08\text{s}^{-1}}{0.42\text{s}^{-1}}\right)^{\frac{1}{2}}\right) + 1\right)^2}$$

13) 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 $$54.15527\text{mol/m}^3 = 80\text{mol/m}^3 \cdot \left(\frac{0.42\text{s}^{-1}}{0.08\text{s}^{-1}}\right)^{\frac{0.08\text{s}^{-1}}{0.08\text{s}^{-1} - 0.42\text{s}^{-1}}}$$

14) Maximum Intermediate Concentration in First Order followed by Zero Order Reaction

Open Calculator

fx $$C_{R,max} = C_{A0} \cdot \left(1 - \left(\frac{k_0}{C_{A0} \cdot k_I} \cdot \left(1 - \ln\left(\frac{k_0}{C_{A0} \cdot k_I}\right)\right)\right)\right)$$

ex $$39.1007\text{mol/m}^3 = 80\text{mol/m}^3 \cdot \left(1 - \left(\frac{6.5\text{mol/m}^3\text{*s}}{80\text{mol/m}^3 \cdot 0.42\text{s}^{-1}} \cdot \left(1 - \ln\left(\frac{6.5\text{mol/m}^3\text{*s}}{80\text{mol/m}^3 \cdot 0.42\text{s}^{-1}}\right)\right)\right)\right)$$

15) 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 $$32.69631\text{mol/m}^3 = \frac{80\text{mol/m}^3 \cdot 0.42\text{s}^{-1} \cdot 0.08\text{s}^{-1} \cdot \left((12\text{s})^2\right)}{(1 + (0.42\text{s}^{-1} \cdot 12\text{s})) \cdot (1 + (0.08\text{s}^{-1} \cdot 12\text{s}))}$$

16) Rate Constant for First Order Reaction in First Order followed by Zero Order Reaction

Open Calculator

fx $$k_I = \left(\frac{1}{\Delta t}\right) \cdot \ln\left(\frac{C_{A0}}{C_{k0}}\right)$$

ex $$0.401324\text{s}^{-1} = \left(\frac{1}{3\text{s}}\right) \cdot \ln\left(\frac{80\text{mol/m}^3}{24\text{mol/m}^3}\right)$$

17) Rate Constant for First Order Reaction using Rate Constant for Zero Order Reaction

Open Calculator

fx $$k_I = \left(\frac{1}{\Delta t}\right) \cdot \ln\left(\frac{C_{A0}}{C_{A0} - (k_0 \cdot \Delta t) - C_R}\right)$$

ex $$0.153351\text{s}^{-1} = \left(\frac{1}{3\text{s}}\right) \cdot \ln\left(\frac{80\text{mol/m}^3}{80\text{mol/m}^3 - (6.5\text{mol/m}^3\text{*s} \cdot 3\text{s}) - 10\text{mol/m}^3}\right)$$

18) 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 $$0.278458\text{s}^{-1} = \frac{1}{0.08\text{s}^{-1} \cdot \left((6.7\text{s})^2\right)}$$

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

Open Calculator

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

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

20) Rate Constant for Zero Order Reaction using Rate Constant for First Order Reaction

Open Calculator

fx $$k_{0,k1} = \left(\frac{C_{A0}}{\Delta t}\right) \cdot \left(1 - \exp((-k_I) \cdot \Delta t) - \left(\frac{C_R}{C_{A0}}\right)\right)$$

ex $$15.76923\text{mol/m}^3\text{*s} = \left(\frac{80\text{mol/m}^3}{3\text{s}}\right) \cdot \left(1 - \exp((-0.42\text{s}^{-1}) \cdot 3\text{s}) - \left(\frac{10\text{mol/m}^3}{80\text{mol/m}^3}\right)\right)$$

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

Open Calculator

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

ex $$13.24503 \text{mol/m³} = \frac{80 \text{mol/m³}}{1 + (0.42 \text{s}^{-1} \cdot 12 \text{s})}$$

22) Reactant Concentration in First Order followed by Zero Order Reaction

Open Calculator

fx $$C_{k0} = C_{A0} \cdot \exp(-k_I \cdot \Delta t)$$

ex $$22.69232 \text{mol/m³} = 80 \text{mol/m³} \cdot \exp(-0.42 \text{s}^{-1} \cdot 3 \text{s})$$

23) Time at Max Intermediate in First Order followed by Zero Order Reaction

Open Calculator

fx $$\tau_{R,max} = \left(\frac{1}{k_I}\right) \cdot \ln\left(\frac{k_I \cdot C_{A0}}{k_0}\right)$$

ex $$3.911247 \text{s} = \left(\frac{1}{0.42 \text{s}^{-1}}\right) \cdot \ln\left(\frac{0.42 \text{s}^{-1} \cdot 80 \text{mol/m³}}{6.5 \text{mol/m³*s}}\right)$$

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

Open Calculator

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

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

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

Open Calculator

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

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

26) Time Interval for First Order Reaction in First Order followed by Zero Order Reaction

Open Calculator

$$\Delta t = \left(\frac{1}{k_I}\right) \cdot \ln\left(\frac{C_{A0}}{C_{k0}}\right)$$

$$2.866602\text{s} = \left(\frac{1}{0.42\text{s}^{-1}}\right) \cdot \ln\left(\frac{80\text{mol/m}^3}{24\text{mol/m}^3}\right)$$

Variables Used

- **$C_{A0 \text{ for } R}$** Initial Reactant Concentration using Intermediate *(Mole per Cubic Meter)*
- **C_{A0}** Initial Reactant Concentration for Multiple Rxns *(Mole per Cubic Meter)*
- **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_{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** Intermediate Concentration for Series Rxn *(Mole per Cubic Meter)*
- **$C_{R,1st\ order}$** Intermediate Conc. for 1st Order Series Rxn *(Mole per Cubic Meter)*
- **$C_{R,max}$** Maximum Intermediate Concentration *(Mole per Cubic Meter)*
- **$C_{R,max}$** Maximum Intermediate Concentration *(Mole per Cubic Meter)*
- **C_S** Final Product Concentration *(Mole per Cubic Meter)*
- **k_0** Rate Constant for Zero Order Rxn for Multiple Rxns *(Mole per Cubic Meter Second)*
- **$k_{0,k1}$** Rate Constant for Zero Order Rxn using k1 *(Mole per Cubic Meter Second)*
- **k_2** Rate Constant for Second Step First Order Reaction *(1 Per Second)*
- **k_I** Rate Constant for First Step First Order Reaction *(1 Per Second)*
- **k_I** Rate Constant for First Step First Order Reaction *(1 Per Second)*
- **Δt** Time Interval for Multiple Reactions *(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)*
- **$\tau_{R,max}$** Time at Maximum Intermediate Concentration *(Second)*

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/m^3)
  Molar Concentration 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

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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