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Reactor Performance Equations for Variable Volume Reactions Formulas

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List of 17 Reactor Performance Equations for Variable Volume Reactions Formulas

Reactor Performance Equations for Variable Volume Reactions

1) Initial Reactant Concentration for Second Order Reaction for Mixed Flow

$$C_{O_{\text{MixedFlow}}} = \left(\frac{1}{\tau_{\text{MFR}}} \cdot k''^{\text{MFR}} \right) \cdot \left(\frac{X_{\text{MFR}} \cdot (1 + (\varepsilon \cdot X_{\text{MFR}}))^2}{(1 - X_{\text{MFR}})^2} \right)$$

[Open Calculator !\[\]\(a870788d6ed9b8fd294b7654a8c8526b_img.jpg\)](#)

$$\text{ex } 10.32254 \text{ mol/m}^3 = \left(\frac{1}{0.0612 \text{ s}} \cdot 0.0607 \text{ m}^3 / (\text{mol} \cdot \text{s}) \right) \cdot \left(\frac{0.702 \cdot (1 + (0.21 \cdot 0.702))^2}{(1 - 0.702)^2} \right)$$

2) Initial Reactant Concentration for Second Order Reaction for Plug Flow

$$C_{O_{\text{PlugFlow}}} = \left(\frac{1}{\tau_{\text{pfr}} \cdot k''} \right) \cdot \left(2 \cdot \varepsilon_{\text{PFR}} \cdot (1 + \varepsilon_{\text{PFR}}) \cdot \ln(1 - X_{\text{A-PFR}}) + \varepsilon_{\text{PFR}}^2 \cdot X_{\text{A-PFR}} + \left(\varepsilon_{\text{PFR}} \right) \right)$$

[Open Calculator !\[\]\(c50c8b7b2cc2cf9ff925edec0ee94c0d_img.jpg\)](#)

$$\text{ex } 1016.209 \text{ mol/m}^3 = \left(\frac{1}{0.05009 \text{ s} \cdot 0.0608 \text{ m}^3 / (\text{mol} \cdot \text{s})} \right) \cdot \left(2 \cdot 0.22 \cdot (1 + 0.22) \cdot \ln(1 - 0.715) + (0.22)^2 \cdot 0.715 + 0.22 \right)$$

3) Initial Reactant Concentration for Zero Order Reaction for Mixed Flow

$$C_{O_{\text{-MFR}}} = \frac{k_{0\text{-MFR}} \cdot \tau_{\text{MFR}}}{X_{\text{MFR}}}$$

[Open Calculator !\[\]\(f60b7a900783ac3fd531bfd9c111be6d_img.jpg\)](#)

$$\text{ex } 89.01026 \text{ mol/m}^3 = \frac{1021 \text{ mol/m}^3 \cdot \text{s} \cdot 0.0612 \text{ s}}{0.702}$$

4) Initial Reactant Concentration for Zero Order Reaction for Plug Flow

$$C_{O_{\text{pfr}}} = \frac{k_0 \cdot \tau_{\text{pfr}}}{X_{\text{A-PFR}}}$$

[Open Calculator !\[\]\(83bbbd261710c59db0214aa27b2edc0d_img.jpg\)](#)

$$\text{ex } 78.46266 \text{ mol/m}^3 = \frac{1120 \text{ mol/m}^3 \cdot \text{s} \cdot 0.05009 \text{ s}}{0.715}$$



5) Rate Constant for First Order Reaction for Mixed Flow 

$$k_{1\text{MFR}} = \left(\frac{1}{\tau_{\text{MFR}}} \right) \cdot \left(\frac{X_{\text{MFR}} \cdot (1 + (\varepsilon \cdot X_{\text{MFR}}))}{1 - X_{\text{MFR}}} \right)$$

Open Calculator 

$$\text{ex } 44.16638\text{s}^{-1} = \left(\frac{1}{0.0612\text{s}} \right) \cdot \left(\frac{0.702 \cdot (1 + (0.21 \cdot 0.702))}{1 - 0.702} \right)$$

6) Rate Constant for First Order Reaction for Plug Flow 

$$k_{\text{plug flow}} = \left(\frac{1}{\tau_{\text{pfr}}} \right) \cdot \left((1 + \varepsilon_{\text{PFR}}) \cdot \ln \left(\frac{1}{1 - X_{\text{A-PFR}}} \right) - (\varepsilon_{\text{PFR}} \cdot X_{\text{A-PFR}}) \right)$$

Open Calculator 


$$\text{ex } 27.43311\text{s}^{-1} = \left(\frac{1}{0.05009\text{s}} \right) \cdot \left((1 + 0.22) \cdot \ln \left(\frac{1}{1 - 0.715} \right) - (0.22 \cdot 0.715) \right)$$

7) Rate Constant for Second Order Reaction for Mixed Flow 

$$k^{\text{MixedFlow}} = \left(\frac{1}{\tau_{\text{MFR}} \cdot C_{\text{o-MFR}}} \right) \cdot \left(\frac{X_{\text{MFR}} \cdot (1 + (\varepsilon \cdot X_{\text{MFR}}))^2}{(1 - X_{\text{MFR}})^2} \right)$$

Open Calculator 

$$\text{ex } 13774.73\text{m}^3/(\text{mol} \cdot \text{s}) = \left(\frac{1}{0.0612\text{s}} \cdot 81\text{mol}/\text{m}^3 \right) \cdot \left(\frac{0.702 \cdot (1 + (0.21 \cdot 0.702))^2}{(1 - 0.702)^2} \right)$$

8) Rate Constant for Second Order Reaction for Plug Flow 

$$k^{\text{PlugFlow}} = \left(\frac{1}{\tau \cdot C_{\text{o}}} \right) \cdot \left(2 \cdot \varepsilon \cdot (1 + \varepsilon) \cdot \ln(1 - X_{\text{A}}) + \varepsilon^2 \cdot X_{\text{A}} + \left((\varepsilon + 1)^2 \cdot \frac{X_{\text{A}}}{1 - X_{\text{A}}} \right) \right)$$

Open Calculator 

$$\text{ex } 0.708811\text{m}^3/(\text{mol} \cdot \text{s}) = \left(\frac{1}{0.05\text{s} \cdot 80\text{mol}/\text{m}^3} \right) \cdot \left(2 \cdot 0.21 \cdot (1 + 0.21) \cdot \ln(1 - 0.7) + (0.21)^2 \cdot 0.7 + \left((0.21 + 1)^2 \cdot \frac{0.7}{1 - 0.7} \right) \right)$$

9) Rate Constant for Zero Order Reaction for Mixed Flow 

$$k_{\text{0-MFR}} = \frac{X_{\text{MFR}} \cdot C_{\text{o-MFR}}}{\tau_{\text{MFR}}}$$

Open Calculator 

$$\text{ex } 929.1176\text{mol}/\text{m}^3 \cdot \text{s} = \frac{0.702 \cdot 81\text{mol}/\text{m}^3}{0.0612\text{s}}$$




10) Rate Constant for Zero Order Reaction for Plug Flow 

$$\text{fx } k_0 = \frac{X_{A\text{-PFR}} \cdot C_{o\text{ pfr}}}{\tau_{\text{pfr}}}$$

Open Calculator 


$$\text{ex } 1170.493 \text{ mol/m}^3 \cdot \text{s} = \frac{0.715 \cdot 82 \text{ mol/m}^3}{0.05009 \text{ s}}$$

11) Reactant Conversion for Zero Order Reaction for Mixed Flow 

$$\text{fx } X_{\text{MFR}} = \frac{k_{0\text{-MFR}} \cdot \tau_{\text{MFR}}}{C_{o\text{-MFR}}}$$

Open Calculator 


$$\text{ex } 0.771422 = \frac{1021 \text{ mol/m}^3 \cdot \text{s} \cdot 0.0612 \text{ s}}{81 \text{ mol/m}^3}$$

12) Reactant Conversion for Zero Order Reaction for Plug Flow 

$$\text{fx } X_{A\text{-PFR}} = \frac{k_0 \cdot \tau_{\text{pfr}}}{C_{o\text{ pfr}}}$$

Open Calculator 


$$\text{ex } 0.684156 = \frac{1120 \text{ mol/m}^3 \cdot \text{s} \cdot 0.05009 \text{ s}}{82 \text{ mol/m}^3}$$

13) Space Time for First Order Reaction using Rate Constant for Mixed Flow 

$$\text{fx } \tau_{\text{MFR}} = \left(\frac{1}{k_{1\text{MFR}}} \right) \cdot \left(\frac{X_{\text{MFR}} \cdot (1 + (\varepsilon \cdot X_{\text{MFR}}))}{1 - X_{\text{MFR}}} \right)$$

Open Calculator 

$$\text{ex } 0.068257 \text{ s} = \left(\frac{1}{39.6 \text{ s}^{-1}} \right) \cdot \left(\frac{0.702 \cdot (1 + (0.21 \cdot 0.702))}{1 - 0.702} \right)$$


14) Space Time for First Order Reaction using Rate Constant for Plug Flow 

$$\text{fx } \tau_{\text{pfr}} = \left(\frac{1}{k_{\text{plug flow}}} \right) \cdot \left((1 + \varepsilon_{\text{PFR}}) \cdot \ln \left(\frac{1}{1 - X_{A\text{-PFR}}} \right) - (\varepsilon_{\text{PFR}} \cdot X_{A\text{-PFR}}) \right)$$

Open Calculator 


$$\text{ex } 0.034788 \text{ s} = \left(\frac{1}{39.5 \text{ s}^{-1}} \right) \cdot \left((1 + 0.22) \cdot \ln \left(\frac{1}{1 - 0.715} \right) - (0.22 \cdot 0.715) \right)$$



15) Space Time for Second Order Reaction using Rate Constant for Mixed Flow [Open Calculator](#) 


$$\text{fx } \tau_{\text{MixedFlow}} = \left(\frac{1}{k''_{\text{MFR}}} \cdot C_{\text{o-MFR}} \right) \cdot \left(\frac{X_{\text{MFR}} \cdot (1 + (\varepsilon \cdot X_{\text{MFR}}))^2}{(1 - X_{\text{MFR}})^2} \right)$$

$$\text{ex } 13888.19\text{s} = \left(\frac{1}{0.0607\text{m}^3/(\text{mol}\cdot\text{s})} \cdot 81\text{mol}/\text{m}^3 \right) \cdot \left(\frac{0.702 \cdot (1 + (0.21 \cdot 0.702))^2}{(1 - 0.702)^2} \right)$$

16) Space Time for Zero Order Reaction using Rate Constant for Mixed Flow [Open Calculator](#) 

$$\text{fx } \tau_{\text{MFR}} = \frac{X_{\text{MFR}} \cdot C_{\text{o-MFR}}}{k_{\text{o-MFR}}}$$

$$\text{ex } 0.055692\text{s} = \frac{0.702 \cdot 81\text{mol}/\text{m}^3}{1021\text{mol}/\text{m}^3\cdot\text{s}}$$

17) Space Time for Zero Order Reaction using Rate Constant for Plug Flow [Open Calculator](#) 

$$\text{fx } \tau_{\text{pfr}} = \frac{X_{\text{A-PFR}} \cdot C_{\text{o pfr}}}{k_0}$$

$$\text{ex } 0.052348\text{s} = \frac{0.715 \cdot 82\text{mol}/\text{m}^3}{1120\text{mol}/\text{m}^3\cdot\text{s}}$$








Variables Used

- $C_{O\ pfr}$ Initial Reactant Concentration in PFR (Mole per Cubic Meter)
- C_O Initial Reactant Concentration (Mole per Cubic Meter)
- C_{O-MFR} Initial Reactant Concentration in MFR (Mole per Cubic Meter)
- $C_{O\ MixedFlow}$ Initial Reactant Conc for 2nd Order Mixed Flow (Mole per Cubic Meter)
- $C_{O\ PlugFlow}$ Initial Reactant Conc for 2nd Order Plug Flow (Mole per Cubic Meter)
- k_0 Rate Constant for Zero Order Reaction (Mole per Cubic Meter Second)
- k_{0-MFR} Rate Constant for Zero Order Reaction in MFR (Mole per Cubic Meter Second)
- $k_{plug\ flow}$ Rate Constant for First Order in Plug Flow (1 Per Second)
- $k''\ MFR$ Rate Constant for Second Order Reaction in MFR (Cubic Meter per Mole Second)
- k'' Rate Constant for Second Order Reaction (Cubic Meter per Mole Second)
- $k^{MixedFlow''}$ Rate Constant for 2nd Order Reaction for Mixed Flow (Cubic Meter per Mole Second)
- $k^{PlugFlow''}$ Rate Constant for 2nd Order Reaction for Plug Flow (Cubic Meter per Mole Second)
- k_{1MFR} Rate Constant for First Order Reaction in MFR (1 Per Second)
- X_A Reactant Conversion
- X_{A-PFR} Reactant Conversion in PFR
- X_{MFR} Reactant Conversion in MFR
- ϵ Fractional Volume Change in Reactor
- ϵ Fractional Volume Change
- ϵ_{PFR} Fractional Volume Change in PFR
- τ Space Time (Second)
- τ_{MFR} Space Time in MFR (Second)
- $\tau_{MixedFlow}$ Space Time for Mixed Flow (Second)
- τ_{pfr} Space Time in PFR (Second)














Constants, Functions, Measurements used

- **Function:** **ln**, $\ln(\text{Number})$
Natural logarithm function (base e)
- **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 ($\text{mol}/\text{m}^3\cdot\text{s}$)
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 Cubic Meter per Mole Second ($\text{m}^3/(\text{mol}\cdot\text{s})$)
Second 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](#) 
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