Important Reactor Performance Equations for Variable Volume Reactions Formulas PDF

Formulas Examples with Units

List of 17
Important Reactor Performance Equations for Variable Volume Reactions Formulas

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

Evaluate Formula

Formula

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

Example with Units

$$10.3225 \, \text{mol/m}^3 = \left(\frac{1}{0.0612 \, \text{s}} \cdot 0.0607 \, \text{m}^3\text{/(mol*s)} \right) \cdot \left(\frac{0.702 \cdot \left(1 + \left(0.21 \cdot 0.702 \right) \right)^2}{\left(1 - 0.702 \right)^2} \right)$$

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

Evaluate Formula

Formula

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

Example with Units

$$1016.2088 \, \text{mol/m}^3 = \left(\frac{1}{0.05009 \, \text{s} \cdot 0.0608 \, \text{m}^3\text{/(mol*s)}} \right) \cdot \left(2 \cdot 0.22 \cdot \left(1 + 0.22 \right) \cdot \ln\left(1 - 0.715 \right) + 0.22^2 \cdot 0.715 + \left(\left(0.22 + 1 \right)^2 \cdot \frac{0.715}{1 - 0.715} \right) \right)$$

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

Evaluate Formula

Formula

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

Example with Units

$$89.0103 \, \text{mol/m}^3 = \frac{1021 \, \text{mol/m}^3\text{*s} \cdot 0.0612 \, \text{s}}{0.702}$$

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

Evaluate Formula

Formula

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

Example with Units

$$78.4627 \, \text{mol/m}^3 = \frac{1120 \, \text{mol/m}^3\text{*s} \cdot 0.05009 \, \text{s}}{0.715}$$

5) Rate Constant for First Order Reaction for Mixed Flow Formula

Evaluate Formula

Formula

$$k1_{MFR} = \left(\frac{1}{\tau_{MFR}} \right) \cdot \left(\frac{X_{MFR} \cdot \left(1 + \left(\varepsilon \cdot X_{MFR} \right) \right)}{1 - X_{MFR}} \right)$$

Example with Units

$$44.1664 \, \text{s}^{-1} = \left(\frac{1}{0.0612 \, \text{s}} \right) \cdot \left(\frac{0.702 \cdot \left(1 + \left(0.21 \cdot 0.702 \right) \right)}{1 - 0.702} \right)$$

6) Rate Constant for First Order Reaction for Plug Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$27.4331\,\mathrm{s^{-1}} = \left(\frac{1}{0.05009\,\mathrm{s}}\right) \cdot \left(\left(1 + 0.22\right) \cdot \ln\left(\frac{1}{1 - 0.715}\right) - \left(0.22 \cdot 0.715\right)\right)$$

7) Rate Constant for Second Order Reaction for Mixed Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$13774.7274\,\mathrm{m^3/(mol*s)} = \left(\frac{1}{0.0612\,\mathrm{s}} \cdot 81\,\mathrm{mol/m^3}\right) \cdot \left(\frac{0.702 \cdot \left(1 + \left(0.21 \cdot 0.702\right)\right)^2}{\left(1 - 0.702\right)^2}\right)$$

8) Rate Constant for Second Order Reaction for Plug Flow Formula

Evaluate Formula

Formula

$$k_{PlugFlow''} = \left(\frac{1}{\tau \cdot C_o}\right) \cdot \left(2 \cdot \varepsilon \cdot \left(1 + \varepsilon\right) \cdot \ln\left(1 - X_A\right) + \varepsilon^2 \cdot X_A + \left(\left(\varepsilon + 1\right)^2 \cdot \frac{X_A}{1 - X_A}\right)\right)$$

Example with Units

$$0.7088\,\mathrm{m^3/(mol*s)} = \left(\frac{1}{0.05\,\mathrm{s} \cdot 80\,\mathrm{mol/m^3}}\right) \cdot \left(2 \cdot 0.21 \cdot \left(1 + 0.21\right) \cdot \ln\left(1 - 0.7\right) + 0.21^2 \cdot 0.7 + \left(\left(0.21 + 1\right)^2 \cdot \frac{0.7}{1 - 0.7}\right)\right)$$

9) Rate Constant for Zero Order Reaction for Mixed Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$929.1176\,\mathrm{mol/m^3*s} = \frac{0.702 \cdot 81\,\mathrm{mol/m^3}}{0.0612\,\mathrm{s}}$$

10) Rate Constant for Zero Order Reaction for Plug Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$1170.4931\,\mathrm{mol/m^3*s} = \frac{0.715 \cdot 82\,\mathrm{mol/m^3}}{0.05009\,\mathrm{s}}$$

11) Reactant Conversion for Zero Order Reaction for Mixed Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$0.7714 = \frac{1021\,\mathrm{mol/m^3*s} \cdot 0.0612\,\mathrm{s}}{81\,\mathrm{mol/m^3}}$$

12) Reactant Conversion for Zero Order Reaction for Plug Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$0.6842 = \frac{1120\,\mathrm{mol/m^3*s} \cdot 0.05009\,\mathrm{s}}{82\,\mathrm{mol/m^3}}$$

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

Evaluate Formula

Formula

$$\tau_{MFR} = \left(\frac{1}{k1_{MFR}}\right) \cdot \left(\frac{X_{MFR} \cdot \left(1 + \left(\varepsilon \cdot X_{MFR}\right)\right)}{1 - X_{MFR}}\right)$$

Example with Units

$$0.0683\,\text{s} = \left(\frac{1}{39.6\,\text{s}^{-1}}\right) \cdot \left(\frac{0.702 \cdot \left(1 + \left(0.21 \cdot 0.702\right)\right)}{1 - 0.702}\right)$$

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

Evaluate Formula

Formula

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

Example with Units

$$0.0348\,\text{s} = \left(\frac{1}{39.5\,\text{s}^{-1}}\right) \cdot \left(\left(1 + 0.22\right) \cdot \ln\left(\frac{1}{1 - 0.715}\right) - \left(0.22 \cdot 0.715\right)\right)$$

15) Space Time for Second Order Reaction using Rate Constant for Mixed Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$13888.193\,\text{s} = \left(\frac{1}{0.0607\,\text{m}^3/(\text{mol*s})} \cdot 81\,\text{mol/m}^3\right) \cdot \left(\frac{0.702 \cdot \left(1 + \left(0.21 \cdot 0.702\right)\right)^2}{\left(1 - 0.702\right)^2}\right)$$

16) Space Time for Zero Order Reaction using Rate Constant for Mixed Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0557\,\text{s} = \frac{0.702 \cdot 81\,\text{mol/m}^3}{1021\,\text{mol/m}^3\text{*s}}$$

17) Space Time for Zero Order Reaction using Rate Constant for Plug Flow Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0523\,\text{s} = \frac{0.715 \cdot 82\,\text{mol/m}^3}{1120\,\text{mol/m}^3\text{*s}}$$

Variables used in list of Reactor Performance Equations for Variable Volume Reactions Formulas above

- $C_{o\ pfr}$ Initial Reactant Concentration in PFR *(Mole per Cubic Meter)*
- C_o Initial Reactant Concentration *(Mole per Cubic Meter)*
- $C_{o\text{-}MFR}$ Initial Reactant Concentration in MFR *(Mole per Cubic Meter)*
- $Co_{MixedFlow}$ Initial Reactant Conc for 2nd Order Mixed Flow *(Mole per Cubic Meter)*
- $Co_{PlugFlow}$ 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)*
- $k_{0\text{-}MFR}$ 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 2ndOrder 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)*
- $k1_{MFR}$ Rate Constant for First Order Reaction in MFR *(1 Per Second)*
- X_A Reactant Conversion
- $X_{A\text{-}PFR}$ 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 in list of Reactor Performance Equations for Variable Volume Reactions Formulas above

- 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.
- Measurement: **Time** in Second (s)
  Time Unit Conversion
- Measurement: **Molar Concentration** in Mole per Cubic Meter (mol/m³)
  Molar Concentration 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 Cubic Meter per Mole Second (m³/(mol*s))
  Second Order Reaction Rate Constant Unit Conversion

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