Important Formulas in Design of Reactors & Recycle Reactors for Single Reactions PDF

Formulas Examples with Units

List of 27
Important Formulas in Design of Reactors & Recycle Reactors for Single Reactions

1) Final Reactant Conversion Formula

Evaluate Formula

Formula

$$X_f = \left(\frac{R+1}{R}\right) \cdot X_1$$

Example

$$0.6002 = \left(\frac{0.3+1}{0.3}\right) \cdot 0.1385$$

2) Initial Reactant Concentration for First Order Reaction in Vessel i Formula

Evaluate Formula

Formula

$$C_{i\text{-}1} = C_i \cdot \left(1 + \left(k' \cdot trC2'\right)\right)$$

Example with Units

$$3415.8\,\text{mol/m}^3 = 30\,\text{mol/m}^3 \cdot \left(1 + \left(2.508\,\text{s}^{-1} \cdot 45\,\text{s}\right)\right)$$

3) Initial Reactant Concentration for First Order Reaction using Reaction Rate Formula

Evaluate Formula

Formula

$$C_o = \frac{trC2' \cdot r_i}{X_{i\text{-}1} - X_i}$$

Example with Units

$$76.5\,\text{mol/m}^3 = \frac{45\,\text{s} \cdot 0.17\,\text{mol/m}^3\text{*s}}{0.8 - 0.7}$$

4) Initial Reactant Concentration for Second Order Reaction for Plug Flow or Infinite Reactors Formula

Evaluate Formula

Formula

$$C_o = \frac{1}{\left(\frac{1}{C}\right) - \left(k'' \cdot \tau_p\right)}$$

Example with Units

$$83.9866\,\text{mol/m}^3 = \frac{1}{\left(\frac{1}{24\,\text{mol/m}^3}\right) - \left(0.062\,\text{m}^3\text{/(mol*s)} \cdot 0.48\,\text{s}\right)}$$

5) Rate Constant for First Order Reaction using Recycle Ratio Formula

Evaluate Formula

Formula

$$k' = \left(\frac{R+1}{\tau}\right) \cdot \ln\left(\frac{C_o + \left(R \cdot C_f\right)}{\left(R+1\right) \cdot C_f}\right)$$

Example with Units

$$31.1025\,\text{s}^{-1} = \left(\frac{0.3+1}{0.05\,\text{s}}\right) \cdot \ln\left(\frac{80\,\text{mol/m}^3 + \left(0.3 \cdot 20\,\text{mol/m}^3\right)}{\left(0.3+1\right) \cdot 20\,\text{mol/m}^3}\right)$$

6) Rate Constant for Second Order Reaction using Recycle Ratio Formula

Evaluate Formula

Formula

$$k'' = \frac{(R+1) \cdot C_o \cdot (C_o - C_f)}{C_o \cdot \tau \cdot C_f \cdot (C_o + (R \cdot C_f))}$$

Example with Units

$$0.907\,\text{m}^3/(\text{mol*s}) = \frac{(0.3+1) \cdot 80\,\text{mol/m}^3 \cdot (80\,\text{mol/m}^3 - 20\,\text{mol/m}^3)}{80\,\text{mol/m}^3 \cdot 0.05\,\text{s} \cdot 20\,\text{mol/m}^3 \cdot (80\,\text{mol/m}^3 + (0.3 \cdot 20\,\text{mol/m}^3))}$$

7) Reactant Concentration for First Order Reaction in Vessel i Formula

Evaluate Formula

Formula

$$C_i = \frac{C_{i-1}}{1 + (k' \cdot trC2')}$$

Example with Units

$$0.4391\,\text{mol/m}^3 = \frac{50\,\text{mol/m}^3}{1 + (2.508\,\text{s}^{-1} \cdot 45\,\text{s})}$$

8) Reactant Concentration for Second Order Reaction for Plug Flow or Infinite Reactors Formula

Evaluate Formula

Formula

$$C = \frac{C_o}{1 + (C_o \cdot k'' \cdot \tau_p)}$$

Example with Units

$$23.663\,\text{mol/m}^3 = \frac{80\,\text{mol/m}^3}{1 + (80\,\text{mol/m}^3 \cdot 0.062\,\text{m}^3/(\text{mol*s}) \cdot 0.48\,\text{s})}$$

9) Reaction Rate for Vessel i for Mixed Flow Reactors of Different Sizes in Series Formula

Evaluate Formula

Formula

$$r_i = \frac{C_{i-1} - C_i}{trC2'}$$

Example with Units

$$0.4444\,\text{mol/m}^3\text{*s} = \frac{50\,\text{mol/m}^3 - 30\,\text{mol/m}^3}{45\,\text{s}}$$

10) Recycle Ratio Formula

Evaluate Formula

Formula

$$R = \frac{V_R}{V_D}$$

Example with Units

$$0.3 = \frac{40\,\text{m}^3}{133.33\,\text{m}^3}$$

11) Recycle Ratio using Reactant Conversion Formula

Evaluate Formula

Formula

$$R = \frac{1}{\left(\frac{X_f}{X_1}\right) - 1}$$

Example

$$0.3001 = \frac{1}{\left(\frac{0.6}{0.1385}\right) - 1}$$

12) Recycle Ratio using Total Feed Rate Formula

Evaluate Formula

Formula

$$R = \left(\frac{F0'}{F}\right) - 1$$

Example with Units

$$0.25 = \left(\frac{15\,\text{mol/s}}{12\,\text{mol/s}}\right) - 1$$

13) Space Time for First Order Reaction for Plug Flow or for Infinite Reactors Formula

Evaluate Formula

Formula

$$\tau_p = \left(\frac{1}{k'}\right) \cdot \ln\left(\frac{C_o}{C}\right)$$

Example with Units

$$0.4801\,\text{s} = \left(\frac{1}{2.508\,\text{s}^{-1}}\right) \cdot \ln\left(\frac{80\,\text{mol/m}^3}{24\,\text{mol/m}^3}\right)$$

14) Space Time for First Order Reaction for Vessel i using Molar Flow Rate Formula

Evaluate Formula

Formula

$$trC2' = \frac{V_i \cdot C_o}{F_0}$$

Example with Units

$$48\,\text{s} = \frac{3\,\text{m}^3 \cdot 80\,\text{mol/m}^3}{5\,\text{mol/s}}$$

15) Space Time for First Order Reaction for Vessel i using Reaction Rate Formula

Evaluate Formula

Formula

$$trC2' = \frac{C_o \cdot \left(X_{i-1} - X_i\right)}{r_i}$$

Example with Units

$$47.0588\,\text{s} = \frac{80\,\text{mol/m}^3 \cdot \left(0.8 - 0.7\right)}{0.17\,\text{mol/m}^3\text{*s}}$$

16) Space Time for First Order Reaction for Vessel i using Volumetric Flow Rate Formula

Evaluate Formula

Formula

$$trC2' = \frac{V_i}{\upsilon}$$

Example with Units

$$49.1803\,\text{s} = \frac{3\,\text{m}^3}{0.061\,\text{m}^3\text{/s}}$$

17) Space Time for First Order Reaction in Vessel i Formula

Evaluate Formula

Formula

$$trC2' = \frac{C_{i-1} - C_i}{C_i \cdot k'}$$

Example with Units

$$0.2658\,\text{s} = \frac{50\,\text{mol/m}^3 - 30\,\text{mol/m}^3}{30\,\text{mol/m}^3 \cdot 2.508\,\text{s}^{-1}}$$

18) Space Time for First Order Reaction using Recycle Ratio Formula

Evaluate Formula

Formula

$$\tau = \left(\frac{R+1}{k'}\right)\cdot\ln\left(\frac{C_o + (R\cdot C_f)}{(R+1)\cdot C_f}\right)$$

Example with Units

$$0.6201\,\mathrm{s} = \left(\frac{0.3+1}{2.508\,\mathrm{s^{-1}}}\right)\cdot\ln\left(\frac{80\,\mathrm{mol/m^3} + (0.3\cdot 20\,\mathrm{mol/m^3})}{(0.3+1)\cdot 20\,\mathrm{mol/m^3}}\right)$$

19) Space Time for Second Order Reaction for Plug Flow or Infinite Reactors Formula

Evaluate Formula

Formula

$$\tau_p = \left(\frac{1}{C_o\cdot k''}\right)\cdot\left(\left(\frac{C_o}{C}\right)-1\right)$$

Example with Units

$$0.4704\,\mathrm{s} = \left(\frac{1}{80\,\mathrm{mol/m^3}\cdot 0.062\,\mathrm{m^3/(mol*s)}}\right)\cdot\left(\left(\frac{80\,\mathrm{mol/m^3}}{24\,\mathrm{mol/m^3}}\right)-1\right)$$

20) Space Time for Second Order Reaction using Recycle Ratio Formula

Evaluate Formula

Formula

$$\tau = \frac{(R+1)\cdot C_o\cdot(C_o - C_f)}{C_o\cdot k''\cdot C_f\cdot(C_o + (R\cdot C_f))}$$

Example with Units

$$0.7314\,\mathrm{s} = \frac{(0.3+1)\cdot 80\,\mathrm{mol/m^3}\cdot(80\,\mathrm{mol/m^3} - 20\,\mathrm{mol/m^3})}{80\,\mathrm{mol/m^3}\cdot 0.062\,\mathrm{m^3/(mol*s)}\cdot 20\,\mathrm{mol/m^3}\cdot(80\,\mathrm{mol/m^3} + (0.3\cdot 20\,\mathrm{mol/m^3}))}$$

21) Space Time for Vessel i for Mixed Flow Reactors of Different Sizes in Series Formula

Evaluate Formula

Formula

$$trC2' = \frac{C_{i-1} - C_i}{r_i}$$

Example with Units

$$117.6471\,\mathrm{s} = \frac{50\,\mathrm{mol/m^3} - 30\,\mathrm{mol/m^3}}{0.17\,\mathrm{mol/m^3*s}}$$

22) Total Feed Reactant Conversion Formula

Evaluate Formula

Formula

$$X_1 = \left(\frac{R}{R+1}\right)\cdot X_f$$

Example

$$0.1385 = \left(\frac{0.3}{0.3+1}\right)\cdot 0.6$$

23) Volume leaving System Formula

Evaluate Formula

Formula

$$V_D = \frac{V_R}{R}$$

Example with Units

$$133.3333\,m^3 = \frac{40\,m^3}{0.3}$$

24) Volume of Fluid returned to Reactor Entrance Formula

Evaluate Formula

Formula

$$V_R = V_D \cdot R$$

Example with Units

$$39.999\,m^3 = 133.33\,m^3 \cdot 0.3$$

25) Volume of Vessel i for First Order Reaction using Molar Feed Rate Formula

Evaluate Formula

Formula

$$V_i = \frac{trC2' \cdot F_0}{C_o}$$

Example with Units

$$2.8125\,m^3 = \frac{45\,s \cdot 5\,mol/s}{80\,mol/m^3}$$

26) Volume of Vessel i for First Order Reaction using Volumetric Flow Rate Formula

Evaluate Formula

Formula

$$V_i = \upsilon \cdot trC2'$$

Example with Units

$$2.745\,m^3 = 0.061\,m^3/s \cdot 45\,s$$

27) Volumetric Flow Rate for First Order Reaction for Vessel i Formula

Evaluate Formula

Formula

$$\upsilon = \frac{V_i}{trC2'}$$

Example with Units

$$0.0667\,m^3/s = \frac{3\,m^3}{45\,s}$$

Variables used in list of Important Formulas in Design of Reactors & Recycle Reactors for Single Reactions above

- **C** Reactant Concentration *(Mole per Cubic Meter)*
- C_{i-1} Reactant Concentration in Vessel i-1 *(Mole per Cubic Meter)*
- C_f Final Reactant Concentration *(Mole per Cubic Meter)*
- C_i Reactant Concentration in Vessel i *(Mole per Cubic Meter)*
- C_o Initial Reactant Concentration *(Mole per Cubic Meter)*
- **F** Fresh Molar Feed Rate *(Mole per Second)*
- F_0 Molar Feed Rate *(Mole per Second)*
- $F0'$ Total Molar Feed Rate *(Mole per Second)*
- k' Rate Constant for First Order Reaction *(1 Per Second)*
- k'' Rate Constant for Second Order Reaction *(Cubic Meter per Mole Second)*
- **R** Recycle Ratio
- r_i Reaction Rate for Vessel i *(Mole per Cubic Meter Second)*
- $trC2'$ Adjusted Retention Time of Comp 2 *(Second)*
- V_D Volume Discharged *(Cubic Meter)*
- V_i Volume of Vessel i *(Cubic Meter)*
- V_R Volume Returned *(Cubic Meter)*
- X_1 Total Feed Reactant Conversion
- X_f Final Reactant Conversion
- X_i Reactant Conversion of Vessel i
- X_{i-1} Reactant Conversion of Vessel i-1
- **υ** Volumetric Flow Rate *(Cubic Meter per Second)*
- **τ** Space Time *(Second)*
- τ_p Space Time for Plug Flow Reactor *(Second)*

Constants, Functions, Measurements used in list of Important Formulas in Design of Reactors & Recycle Reactors for Single Reactions 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: **Volume** in Cubic Meter (m^3)
  Volume Unit Conversion
- Measurement: **Volumetric Flow Rate** in Cubic Meter per Second (m^3/s)
  Volumetric Flow Rate Unit Conversion
- Measurement: **Molar Flow Rate** in Mole per Second (mol/s)
  Molar Flow Rate 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
- Measurement: **Second Order Reaction Rate Constant** in Cubic Meter per Mole Second ($m^3/(mol*s)$)
  Second Order Reaction Rate Constant Unit Conversion