

Heterogeneous Catalytic Reaction

Spoken Tutorial Project
<https://spoken-tutorial.org>

National Mission on Education through ICT
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Learning Objectives



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- **Define a Heterogeneous Catalytic Reaction (HCR)**



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- Define parameters for Plug Flow Reactor required to simulate a HCR



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In this tutorial, we will learn to:

- Define a Heterogeneous Catalytic Reaction (HCR)
- Define parameters for Plug Flow Reactor required to simulate a HCR
- Calculate Conversion and Residence time for HCR in a PFR



System Requirement



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- **DWSIM v 5.6 (Classic UI) Update 8**



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- DWSIM v 5.6 (Classic UI) Update 8
- Windows 10



System Requirement

- DWSIM v 5.6 (Classic UI) Update 8
- Windows 10
- Any OS: Linux, Mac OS X or FOSSEE OS on ARM



Prerequisites



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To practice this tutorial, you should know to



Prerequisites

To practice this tutorial, you should know to

- **Add components to a flowsheet**



Prerequisites

To practice this tutorial, you should know to

- Add components to a flowsheet
- **Select thermodynamic packages**



Prerequisites

To practice this tutorial, you should know to

- Add components to a flowsheet
- Select thermodynamic packages
- Add material and energy streams and specify their properties



Prerequisite Tutorials and Files

- <https://spoken-tutorial.org>



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- <https://spoken-tutorial.org>
- You can access these tutorials and all the associated files from this site



Reaction and Inlet Condition

Reaction	$\text{CH}_4 + \text{H}_2\text{O} \rightleftharpoons 3\text{H}_2 + \text{CO}$	
Package	Peng Robinson	
Dimensions	Volume: 1 m³	Length: 1 m
Inlet Stream	Mass Flow Temperature Pressure Mole Fraction	300 kg/h 730 °C 1.01325 bar $x_{\text{CH}_4} = 0.4975$ $x_{\text{H}_2\text{O}} = 0.4975$ $x_{\text{H}_2} = 0.005$



Catalyst Properties and Gas Constant

- Loading: 0.386 kg/m^3
- Particle Diameter: 0.002 m
- Void Fraction: 0.4
- Gas Constant (R): 8.314 J/mol-K



Reaction Rate and Coefficients

$$R_1 = \frac{\frac{k_1}{P_{H_2}^{2.5}} [P_{CH_4} P_{H_2O} - \frac{P_{H_2}^3 P_{CO}}{K_1}]}{DEN^2}$$

$$k_1 = 4.22 \times 10^{15} \exp\left(\frac{-240100}{RT}\right)$$

$$K_1 = \exp\left(30.42 - \frac{27106}{T}\right)$$

$$DEN = 1 + K_{CH_4} P_{CH_4} + K_{CO} P_{CO} + K_{H_2} P_{H_2} + \frac{K_{H_2O} P_{H_2O}}{P_{H_2}}$$



Reaction Rate Coefficients

$$K_{\text{CH}_4} = 6.65 \times 10^{-4} \exp\left(\frac{38280}{RT}\right)$$

$$K_{\text{H}_2\text{O}} = 1.77 \times 10^5 \exp\left(\frac{-88680}{RT}\right)$$

$$K_{\text{H}_2} = 6.12 \times 10^{-9} \exp\left(\frac{82900}{RT}\right)$$

$$K_{\text{CO}} = 8.23 \times 10^{-5} \exp\left(\frac{70650}{RT}\right)$$



Variables for Partial Pressure



Variables for Partial Pressure

- **Reactants: R**



Variables for Partial Pressure

- Reactants: R
- P_{CH_4} : R1, $P_{\text{H}_2\text{O}}$: R2



Variables for Partial Pressure

- Reactants: R
- P_{CH_4} : R1, $P_{\text{H}_2\text{O}}$: R2
- Products: P



Variables for Partial Pressure

- Reactants: **R**
- P_{CH_4} : **R1**, $P_{\text{H}_2\text{O}}$: **R2**
- Products: **P**
- P_{H_2} : **P1**, P_{CO} : **P2**



Reaction Rate Numerator

$$\text{Numerator of } R_1 = \frac{k_1}{P_{H_2}^{2.5}} [P_{CH_4} P_{H_2O} - \frac{P_{H_2}^3 P_{CO}}{K_1}]$$



Reaction Rate Numerator

$$\begin{aligned}\text{Numerator of } R_1 &= \frac{k_1}{P_{H_2}^{2.5}} \left[P_{CH_4} P_{H_2O} - \frac{P_{H_2}^3 P_{CO}}{K_1} \right] \\ &= \frac{4.22E+15 \exp\left(\frac{-240100}{8.314 \times T}\right)}{(P_1)^{2.5}} \times \left[(R_1 \times R_2) - \frac{(P_1)^3 P_2}{\exp\left(30.42 - \frac{27106}{T}\right)} \right]\end{aligned}$$



Reaction Rate Denominator

$$\text{Denominator of } R_1 = \text{DEN}^2 = \left(1 + K_{\text{CH}_4} P_{\text{CH}_4} + K_{\text{CO}} P_{\text{CO}} + K_{\text{H}_2} P_{\text{H}_2} + \frac{K_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}}}{P_{\text{H}_2}}\right)^2$$



Reaction Rate Denominator

$$\begin{aligned}\text{Denominator of } R_1 &= \text{DEN}^2 = \\ & \left(1 + K_{\text{CH}_4} P_{\text{CH}_4} + K_{\text{CO}} P_{\text{CO}} + K_{\text{H}_2} P_{\text{H}_2} + \frac{K_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}}}{P_{\text{H}_2}}\right)^2 \\ &= \left(1 + 6.65\text{E-}4 \exp\left(\frac{38280}{RT}\right) * R1 + 8.23\text{E-}5 \exp\left(\frac{70650}{RT}\right) * P2 \right. \\ & \quad \left. + 6.12\text{E-}9 \exp\left(\frac{82900}{RT}\right) * P1 + \frac{1.77\text{E+}5 \exp\left(\frac{-88680}{RT}\right) * R2}{P1}\right)^2\end{aligned}$$



Summary

- Define a Heterogeneous Catalytic Reaction (HCR)
- Define parameters for Plug Flow Reactor required to simulate a HCR
- Calculate Conversion and Residence time for HCR in a PFR



Assignment

Water Gas Shift Reaction: $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{CO}_2$

$$R_2 = \frac{\frac{k_2}{P_{\text{H}_2}} [P_{\text{CO}} P_{\text{H}_2\text{O}} - \frac{P_{\text{H}_2} P_{\text{CO}_2}}{K_2}]}{\text{DEN}^2}$$

$$k_2 = 1.96 \times 10^6 \exp\left(\frac{-67130}{RT}\right)$$

$$K_2 = \exp\left(-3.798 + \frac{4160}{T}\right)$$



Assignment

Overall Reaction: $\text{CH}_4 + 2\text{H}_2\text{O} \rightleftharpoons 4\text{H}_2 + \text{CO}_2$

$$R_2 = \frac{\frac{k_3}{P_{\text{H}_2}^{3.5}} [P_{\text{CH}_4} P_{\text{H}_2\text{O}}^2 - \frac{P_{\text{H}_2}^4 P_{\text{CO}_2}}{K_3}]}{\text{DEN}^2}$$

$$k_3 = 1.02 \times 10^5 \exp\left(\frac{-243900}{RT}\right)$$

$$K_3 = \exp\left(34.218 - \frac{31266}{T}\right)$$



About the Spoken Tutorial Project

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The Spoken Tutorial Project Team,

- Conducts workshops using spoken tutorials
- Gives certificates to those who pass an online test
- For more details, please write to contact@spoken-tutorial.org



DWSIM Flowsheeting Project

- The FOSSEE team coordinates conversion of existing flow sheets
- We give honorarium and certificates for those who do this
- For more details, please visit this site
<https://dwsim.fossee.in/flowsheeting-project>



Textbook Companion Project

- The FOSSEE team coordinates coding of solved examples of popular books
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<https://dwsim.fossee.in/textbook-companion-project>



Lab Migration Project

- The FOSSEE team helps migrate commercial simulator labs to DWSIM
- We give honorarium and certificates for those who do this
- For more details, please visit this site
<https://dwsim.fossee.in/lab-migration-project>



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Thanks

- Thanks for joining

