

**PRAIRIE VIEW A&M UNIVERSITY
ROY G. PERRY COLLEGE OF ENGINEERING
DEPARTMENT OF CHEMICAL ENGINEERING
CHEG 3306 Kinetics and Reactor Design, SPRING 2022**

I. COURSE SYLLABUS IN ABET FORMAT

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(Summary of topics can be a separate page or include on the assignment itself)

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

IV. QUIZ

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Original Homework Questions & Master Solution/grading scheme used

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

V. Homework Assignment

Summary of Topics covered by Homework

Original Homework Questions & Master Solution/grading scheme used

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

VI. PROJECT

Summary of Topics Covered by Project

Project Problem Statement and Grading Scheme

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

Course Description in ABET Format

I. COURSE DESCRIPTION IN ABET FORMAT

COURSE SYLLABUS

CHEMICAL ENGINEERING DEPARTMENT

CHEG 3306 Kinetics and Reactor Design

Please use the following format for the course syllabi (2 pages maximum in Times New Roman 12 point font)

1.	Course number and name:	CHEG 3306 Kinetics and Reactor Design
2.	Credits and contact hours:	3 credit hours; 5 contact hours
3.	Instructor's or course coordinator's name:	Dr. Nabila Shamim
4.	Text book: Title:	Elements of Chemical Reaction Engineering,
	Author:	Fogler, H. S.,
	Publisher, Year & Edition:	Prentice-Hall, (6th Edition).
5.	Specific course information	
	a. Brief description of the content of the course (catalog description)	CHEG 3306 Kinetics and Reactor Design, Application of fundamental concepts of reaction stoichiometry, kinetics, and equilibria to the interpretation of reaction rate data. Application of reaction rate, heat, and mass transfer correlations to the design of batch, continuous tank, and tubular reactors. Goals: The goal of this course is to teach students the science and design of reaction engineering processes
	b. Prerequisites or Co-requisites	CHEG 2013 - Materials Science, CHEG 3304 - Chemical Engineering Thermodynamics II MATH 2043 - Differential Equations I
	c. *Indicate whether a required, elective, or selected elective (as per definition provided) course in the program	Required
6.	a. Specific goals for the course specific outcomes of instruction (e.g. The student will be able to explain the significance of current research about a particular topic.) <i>Students will be able to :</i>	b. Explicitly indicate which of the student outcomes listed in Criterion 3 or any other outcomes are addressed by the course. <i>The specific goals for the course specific outcomes listed on the left column will address the following student learning outcomes:</i>
	(i) Identify the limiting reactant, basis of calculation, and excess reactants. (ii) Apply stoichiometric ratios or relative rates and develop a stoichiometric table based on phase and components. (iii) Perform mole balances and energy balances based on chemical reaction and/or reactor type. (iv) Understand reaction mechanisms and reaction pathways.	Outcome 1 An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics.
	(i) Determine the final exit concentration using Excel. (ii) Calculate reactor volume using	

	approximations. (iii) Determine the optimum conversion based on graphs generated in Polymath.	
	(i) Evaluate the selectivity of products in reactions and choose feed location of raw materials. (ii) Increase desired product for single and multiple reactants by selecting appropriate reactor and feed conditions. (iii) Research common safety procedures utilized with different catalytic reactions. Calculation composition or concentration of components entering and leaving reactor. 1. Meet design constraints given in the problem statement.	Outcome 2 An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors..
7	Brief list of topics to be covered	Mole Balances (4 hours) Conversion and Reactor Sizing (6 hours) Rate Laws and Stoichiometry (7 hours) Isothermal Reactor Design (6 hours) Multiple Reactions (6 hours) Catalysis and Catalytic Reactors (6 Hours) Design (6 hours)

***Required** courses are required of all students in the program, **elective** courses (often referred to as open or free electives) are optional for students, and **selected elective** courses are those for which students must take one or more courses from a specified group

Prepared by: Dr. Nabila Shamim

Date: May 16, 2022

II ASSESSMENT RESULTS FOR CURRENT AND PAST THREE PERIODS

Program Outcomes Assessed in this course

Outcome 1:

An ability to identify, formulate, and solve complex engineering problems (CEP) by applying principles of engineering, science, and mathematics.

Outcome 2

An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors..

Assessment Summary of Class Semester Averages for Outcomes (Should be provided for Fall 2019 through Spring 2021 Assessment Period)

Outcomes	1	2
Semester	Semester Class Average (%)	Semester Class Average (%)
Spring 2022	74	91
Spring 2021	74	83
Spring 2020	66	74
Spring 2019	71	85
Comments on Trend of Data (Improving or deteriorating)	Class average is close to the ideal class outcome of 75%. Students came back from online to face to face option. It took some time for students to get adapted.	Average is above the ideal average of 75% The instructor had several one to one meeting and continuously worked with the groups to help them in the projects and technical writing. These helped improve their overall grades.

*Expected Semester Class Average = 70% (or as defined by the program)

Ideal Semester Class Average = 75% (or as defined by the program)

End of Semester Course Assessment Reports Spring 2022 and Last Three Assessment Periods.

Each summary contains the following Information

1. Performance Statistics

- Total number of students in class
- The class average performance (**stated as %**) in each course outcome assessed in this class and the **two previous times course was assessed**.
- The acceptable class average for the class in each outcome area as set by your Department.
- Percentage of students who scored below the expected average in each outcome.

2. Implementation Summary

- Brief summary of plans implemented during the semester based on last assessment report

3. Perceived Problems

- Instructor's **critical evaluation** of perceived problems that affected students' performance. **Realistic problems should be identified throughout the semester and summarized in this section of the report.**

4. New Plans for Addressing Problems

- Instructor's plans for addressing the perceived problems the next time the class is taught. **These should be specific enough for another instructor to implement. Most of these should be things that, you, the instructor can implement to help students to improve. Be creative.**

5. Overall Trend over last three assessment periods

- Instructors summary of overall performance trend for each outcome measured over the last three periods.

5. Were Expectations Met?

- Answer **YES** if the **class average was above the expected average** and the **stated percentage of students** scored at or above the expected average, else answer **NO**.

Table 2.1 END OF SEMESTER COURSE OUTCOME ASSESSMENT REPORT
CHEG 3063-Y01: KINETICS AND REACTOR DESIGN: SRPING 2021 SEMESTER
Report Prepared by: Dr. NABILA SHAMIM Report Date: May 17, 2022

Semester	Analysis Type	Number of Students	Outcome 1.1 Identify and Formulate reaction engineering problems using principles of engineering/mathematics.				Outcome 1.2 1.2 Solve reaction engineering problem using POLYMATH/MATLAB				Outcome 1 Ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science.			
			Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average
Spring 2022	Direct	20	75	70	65	43	75	70	90	100	75	70	74	71
Spring 2021	Hybrid	30	75	70	70	43	75	70	81	83	75	70	74	70
Spring 2020	Direct	23	75	70	56	27	75	70	75	64	75	70	66	27
Implementation Summary		Items implemented from previous report or after meeting previous instructor	1. Students came back to face to face learning. At the beginning they were struggling and achieved lower grade on exam 1. 2. Gradually they did better with problem solving as we did one to one meeting. 3. Students were divided into small group of two with a specific problem to Think-Pair-Share. 4. Discussion topics were assigned in CANVAS helped students to communicate to complete a video submission. Technology used: 5. Surface pro is used to deliver lectures. 6. OneNote software gave the opportunity to write the lecture topics on white page and simultaneously share with students. 7. The split screen option gave the privilege to share the theory and solve the problem side by side. 8. Used active learning and collaboration tools to make the class more interactive. 9. Individually students were assessed using exams and quizzes. 10. . Students' basic concepts on kinetics was analyzed by multiple choice questions.				• Complex engineering assignments were assigned based on Polymath/Matlab • A detail rubric on the project was provided to students				Quizzes, Exams, HWs and were given throughout the semester to formulate and solve complex engineering problems			

Perceived Problems	Perceived problems are directly related to the PC and the sub items under them	Students struggled on developing the CRE algorithms. Poor understanding of Mole balance, Rate laws, stoichiometry	They were unable to effectively apply the information correctly in mole balance, rate laws, and combine them to solve complex problems using polymath. Lack in explaining data obtained by computational tools	Problems were mentioned in the sub-outcomes.
Plans for Addressing Problems	Plans for address specific measures to address PC and their sub areas	The following is recommended for implementation. More tutoring is needed, TA for higher level classes are required.	The instructor provided handouts detailing how to analyze and explain data.	Plans to address problems mentioned in the sub-outcomes
Overall Trend over Periods	Ascertain if there were improvements over previous semesters	Class average and the percentage of students reaching the expected outcome did not meet requirements.	Class average of students reaching the expected outcome and the percentage of students reaching the expected outcome met requirements	Class average of students reaching the expected outcome but the percentage of students reaching the expected outcome did not meet requirements.
Were Expectations Met?	Class Average $\geq 75\%$ and $\geq 70\%$ of Students Performed at or Above Expected Average.	NO	YES	No

END OF SEMESTER COURSE OUTCOME ASSESSMENT REPORT
CHEG 3063-Y01: KINETICS AND REACTOR DESIGN: SRPING 2021 SEMESTER
Report Prepared by: Dr. NABILA SHAMIM Report Date: May 18, 2021

Semester	Analysis Type	Number of Students	Outcome 1.1 Identify and Formulate reaction engineering problems using principles of engineering/mathematics.				Outcome 1.2 1.2 Solve reaction engineering problem using POLYMATH/MATLAB				Outcome 1 Ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science.			
			Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average/	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average
Spring 2021	Hybrid	14	75	70	70	43	75	70	81	83	75	70	74	70
Spring 2020	Direct	23	75	70	56	27	75	70	75	64	75	70	66	27
Implementation Summary		Items implemented from previous report or after meeting previous instructor	1. One of the main issues of online teaching and learning is, it becomes monotonous, so new teaching techniques were adopted to improve teaching with the goal of achieving optimal learning among students. 2. the following techniques and technologies were included: 3. In class we watched short videos and discussed current topics to have some brain breaks and understand safety concerns in reactor design. At the beginning of the class Live Polling was conducted to draw class attention and a quick review of previous class. 2. Students were divided into small breakout room in zoom with a specific problem to Think-Pair-Share. 3. Discussion topics were assigned in CANVAS helped students to know each other better during online classes. They shared thoughts with instructor, peers and made comments. 4. In class we watched short videos and discussed current topics to have some brain breaks. Technology used: 4. Surface pro is used to deliver online lectures. 5. OneNote software gave the opportunity to write the lecture topics on white page and simultaneously share with students. 6. The split screen				- Complex engineering assignments were assigned based on Polymath - Tutorial class were taken to familiarize student with Polymath - A detail rubric on the project was provided to students - Remote access to MATLAB was given to students via VDI. A SOP was provided showing the steps to get remote access. - A detailed SOP shared with student to complete complex problems on multiple reactions.				Quizzes, Exams, HWs and projects were given throughout the semester to formulate and solve complex engineering problems			

		option is a game changer, it gave the privilege to share the theory and solve the problem side by side. 7. Used active learning and collaboration tools to make the class more interactive, polling tool, breakout room and collaborative annotation session. 8. Individually students were assessed using exams and quizzes. 9. Students' basic concepts on kinetics was analyzed by multiple choice questions.		
Perceived Problems	Perceived problems are directly related to the PC and the sub items under them	Students struggled on developing the CRE algorithms. Poor understanding of Mole balance, Rate laws, stoichiometry	They were unable to effectively apply the information correctly in mole balance, rate laws, and combine them to solve complex problems using polymath. Lack in explaining data obtained by computational tools Due to pandemic academic integrity was at risk.	Problems were mentioned in the sub-outcomes.
Plans for Addressing Problems	Plans for address specific measures to address PC and their sub areas	The following is recommended for implementation. More tutoring is needed, TA for higher level classes are required.	The instructor should: Continue providing handouts detailing how to analyze and explain data.	Plans to address problems mentioned in the sub-outcomes
Overall Trend over Periods	Ascertain if there were improvements over previous semesters	Class average and the percentage of students reaching the expected outcome did not meet requirements.	Class average of students reaching the expected outcome and the percentage of students reaching the expected outcome met requirements	Class average of students reaching the expected outcome but the percentage of students reaching the expected outcome did not meet requirements.
Were Expectations Met?	Class Average $\geq 75\%$ and $\geq 70\%$ of Students Performed at or Above Expected Average.	NO	YES	NO

END OF SEMESTER COURSE OUTCOME ASSESSMENT REPORT
CHEG 3306-P01: KINETICS AND REACTOR DESIGN: SRPING 2021 SEMESTER
Report Prepared by: Dr. NABILA SHAMIM Report Date: May 18, 2022

Semester	Analysis Type	Number of Students	Outcome 2.1 Ability to define the kinetics and reactor design Problems				Sub-Outcome 2.2 Ability to Conduct a Review of the Literature				Sub-Outcome 2.3 Ability to perform detailed design of complex chemical engineering design.				Outcome 2 An ability apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors.			
			Expected Class Average	Expected % of student above average	Class Average	% of student above average	Expected Class Average	Expected Percent of students above average	Class Average	% Student meeting Expected Average	Expected Class Average	Expected Percent of students above average	Class Average	% Student meeting Expected Average	Expected Class Average	Expected Percent of students above average	Class Average	% Students meeting Expected Average
Spring 2022	Direct	14	75	70	89	100	75	70	90	100	75	70	92	100	75	70	91	100
Spring 2021	Hybrid	30	75	70	78	83	75	70	85	96	75	70	87	100	75	70	83	93
Implementation Summary	Items implemented from previous report or after meeting previous instructor		Complex engineering assignment to identify and solve reactor design problems such as gas phase reaction with pressure drop, membrane reactor.				New techniques and teaching method were adopted as mentioned earlier. In class we watched safety videos and discussed current topics to have some brain breaks.				- The instructor gave clearer instruction on the design of complex problem. Instructor gave examples of multiple reactions. - Collaborative work on CRE algorithms. Met each groups several times on the progress of the project				the students gathered knowledge on how to use prerequisite information and design a reactor. They learned how to write report and do literature review and gather information to complete the design			
Perceived Problems	Perceived problems are directly related to the PC and the sub items under them		Few Student struggled with developing relative rate laws and combine pressure drop together to develop the design equation.				Students completed the design problems and gather information on catalyst from literature.				- Not all Students were working on the project and were not able to incorporate their knowledge of prerequisites in their work. - It was hard to evaluate individual students. This is one of the reason of higher average was observed for projects				Problems were mentioned in the sub-outcomes.			
Plans for Addressing Problems	Plans for address specific measures to address PC and their sub areas		TA are required to help				TA for higher level classes are required				Hand on reactor system can emphasis the visualization of the project and would help students better understand the design equations and how they are used in the reactor design. Some Individual projects would be helpful to evaluate all student. Plant tours would be good for design purpose				The plans mentioned in the sub-outcomes are recommended.			
Overall Trend over Periods	Ascertain if there were improvements over previous semesters		Class average and expected outcome were significantly high				Class average and expected outcome were significantly high				Class average and expected outcome were significantly high				Average is above the ideal average of 75% The instructor had several one-to-one meeting and continuously worked with the groups to help them in the projects and technical writing. These helped improve their overall grades.			
Were Expectations Met?			YES				YES				YES				YES			

END OF SEMESTER COURSE OUTCOME ASSESSMENT REPORT
CHEG 3063-Y01: KINETICS AND REACTOR DESIGN: SRPING 2021 SEMESTER
Report Prepared by: Dr. NABILA SHAMIM Report Date: May 18, 2021

Semester	Analysis Type	Number of Students	Outcome 2.1 Ability to define the kinetics and reactor design Problems				Sub-Outcome 2.2 Ability to Conduct a Review of the Literature				Sub-Outcome 2.3 Ability to perform detailed design of complex chemical engineering design.				Outcome 2 An ability apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors.			
			Expected Class Average	Expected % of student above average	Class Average	% of student above average	Expected Class Average	Expected Percent of students above average	Class Average	% Student meeting Expected Average	Expected Class Average	Expected Percent of students above average	Class Average	% Student meeting Expected Average	Expected Class Average	Expected Percent of students above average	Class Average	% Student meeting Expected Average
Spring 2021	Hybrid	30	75	70	78	83	75	70	85	96	75	70	87	100	75	70	83	93
Implementation Summary	Items implemented from previous report or after meeting previous instructor		Complex engineering assignment to identify and solve reactor design problems such as gas phase reaction with pressure drop, membrane reactor.				New online techniques and teaching method were adopted as mentioned earlier. Discussion topics were given to conduct literature review. Due to pandemic academic integrity was at risk and project weight was increased.				The instructor gave clearer instruction on the design of complex problem. Instructor gave examples of multiple reactions. Instructor made necessary arrangements to access software remotely. collaborative work on CRE algorithms. Met each groups several times on the progress of the project				the students gathered knowledge on how to use prerequisite information and design a reactor. They learned how to write report and do literature review and gather information to complete the design			
Perceived Problems	Perceived problems are directly related to the PC and the sub items under them		Few Student struggled with developing relative rate laws and combine them together to develop the design equation.				Students struggled with the design problems and gather information from literature				Not all Students were working on the project and were not able to incorporate their knowledge of prerequisites in their work. It was hard to evaluate individual students. This is one of the reason of higher average was observed for projects				Problems were mentioned in the sub-outcomes.			
Plans for Addressing Problems	Plans for address specific measures to address PC and their sub areas		TA are required to help				TA for higher level classes are required				More emphasis should be made on design equations and how they are used in the reactor design. Some Individual projects would be helpful to evaluate all student. Plant tours would be good for design purpose				The plans mentioned in the sub-outcomes are recommended.			
Overall Trend over Periods	Ascertain if there were improvements over previous semesters		Class average and expected outcome were significantly high				Class average and expected outcome were significantly high				Class average and expected outcome were significantly high				Average is above the ideal average of 75% The instructor had several one-to-one meeting and continuously worked with the groups to help them in the projects and technical writing. These helped improve their overall grades.			
Were Expectations Met?			YES				YES				YES				YES			

CHEG 3306-P01: KINETICS AND REACTOR DESIGN

Title of Assignment: EXAM 1

TOPICS COVERED IN EXAM 1

Exam 1 covered the following topics:

1. Mole Balance, Stoichiometry
2. Membrane Reactor, Gas Phase reaction
3. Perform mole balances and energy balances based on chemical reaction and/or reactor type.

CHEG 3306-P01: KINETICS AND REACTOR DESIGN

**SAMPLE TEST QUESTIONS, SOLUTION,
AND GRADING SCHEME FOR MID-TERM EXAM**

Kinetics and Reactor Design CHEG 3306 PO 1

Spring 2022

Exam I Time: 1Hr 20 min Date: March 9 2022

Instructor: Dr. Nabila Shamim

Total points: 100

ABET OUTCOME 1 An ability to identify, formulate and solve complex engineering problem by applying principle of engineering science and mathematics.

STUDENT NAME:DATE:

Competency area	Points	Score earned
Outcome 1.1 Identify and formulate (i) Understand the given problem and identify the subject area and concepts involved Derive mole balance equation rate law and develop stoichiometry table (ii) Formulate the CEP into a mathematical model [using basic, intermediate and advanced mathematics ranging from algebra & trigonometry, calculus Combine all equation to solve for volume	55	
2.1 Solve problems a. Calculate volume, space time, concentration	45	
Total	100	

Closed Book Exam NO CELL PHONE USE (PUT THEM AWAY), NO RESTROOM BREAKS NO COLLABORATION

PROVIDE UNITS ON ALL CALCULATIONS AND ANSWERS

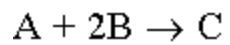
ANY DISHONESTY DURING THE EXAMS WILL RESULT IN "F" GRADE

WORK ALL PROBLEMS ON THE QUESTION SHEETS AND DO NOT USE ANY SHEET OF YOUR OWN

Student Signature:

Problem 1 (15 points)

The following elementary reaction



is carried out in a CSTR. For an entering volumetric flowrate of $10 \text{ dm}^3/\text{s}$ at a concentration of 0.5 mol/dm^3 , what is the space time for the reactor to achieve 90% conversion?

Additional Information: $k_A = 0.01 \text{ mol/dm}^3 \cdot \text{s}$

Problem 2 (30 Points) For the gas phase reaction

Compound A undergoes a reversible isomerization reaction, $A \rightleftharpoons B$, over a supported metal catalyst. Under pertinent conditions, A and B are liquid, miscible, and of nearly identical density; the equilibrium constant for the reaction (in concentration units) is 6.0. In a fixed-bed isothermal flow reactor in which backmixing is negligible (i.e., plug flow), a feed of pure A undergoes a net conversion to B of 50%. The reaction is elementary. If a second, identical flow reactor at the same temperature is placed downstream from the first. The reaction is reversible at constant temperature and pressure.

Follow the CRE algorithms to complete the problem (for example Mole balance equation, Rate laws, Stoichiometry, combine and evaluate etc.)

1. Develop the rate laws
2. Develop the stoichiometric table.
3. Write the concentration of A and B in term of C_{A0} and X .
4. Combine the equations.
5. What overall conversion of A would you expect?

Problem 3 (15 Points) The gas phase irreversible reaction is carried out isothermally in a PBR.



The reaction is zero order. The entering temperature is 400 K, and the entering pressure is 10 atm. The flow is turbulent. For a 10 kg PBR with a pressure drop parameter $\alpha = 0.01 \text{ kg}^{-1}$, the exit conversion was found to be 0.4.

a) What catalyst weight of the PBR will you require if you need an exit conversion of 0.8?

b) **(10 Points)** Assuming that the particle diameter is decreased by a factor of 2 so that the pressure drop parameter α , is now increased to 0.02? Assume all other operating conditions are the same as for the base case (i.e. $W = 10$ kg). For a 10 kg PBR with a pressure drop parameter $\alpha = 0.01 \text{ kg}^{-1}$

For the fixed inlet pressure of 10 atm, will the volumetric flow rate v , (dm^3/s), be greater, smaller, or remain the same when the particle diameter is decreased by a factor of 2?

- a. Increased
- b. Decreased
- c. Remain the same
- d. None of the above

Show your work.

$$v = v_0 (1 + \varepsilon X_A) \left(\frac{Z}{Z_0} \right) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right)$$

$$\boxed{\frac{dp}{dW} = -\frac{\alpha}{2p} (1 + \varepsilon X)} \quad p = (1 - aW)^{1/2}$$

Problem 3 (30 Points)

Problem 3a. (5 Points) Given the following liquid phase reaction and feed conditions what is the correct expression for C_D as a function of the conversion of the limiting reactant X?

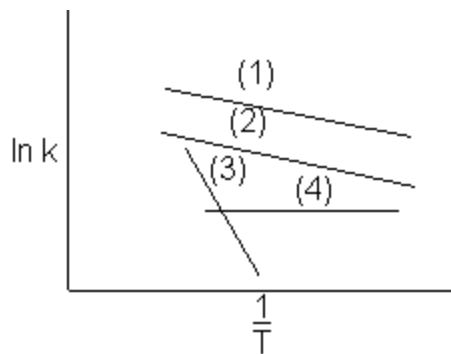


$$C_{A0} = C_{D0} = 1 \text{ mol/min} \quad C_{B0} = 2 \text{ mol/min} \quad C_{C0} = 0$$

- a) $C_D = C_{B0} (1 - X)$
- b) $C_D = C_{B0} (1 + X)$
- c) $C_D = C_{B0} (1 - X/3)$
- d) $C_D = C_{B0} (\frac{1}{2} + X/3)$

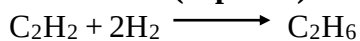
Problem 3b. (5 Points) Consider the following elementary reactions

- 1) $A \xrightarrow{k_1} B$
- 2) $A \xrightarrow{k_2} D$
- 3) $A \xrightarrow{k_3} Y$
- 4) $A \xrightarrow{k_4} U$



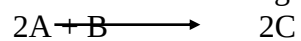
- a) Which reaction has the higher activation energy?
- b) Which reaction is virtually temperature insensitive?

Problem 3c. (5 points) the hydrogenation of acetylene to form ethane



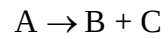
Lets consider 20 Kmol/h acetylene and 50 Kmol/h of hydrogen are fed to the reactor. Which one is the limiting reactant?

Problem 3d. (5 Points) The adiabatic exothermic irreversible gas phase reaction

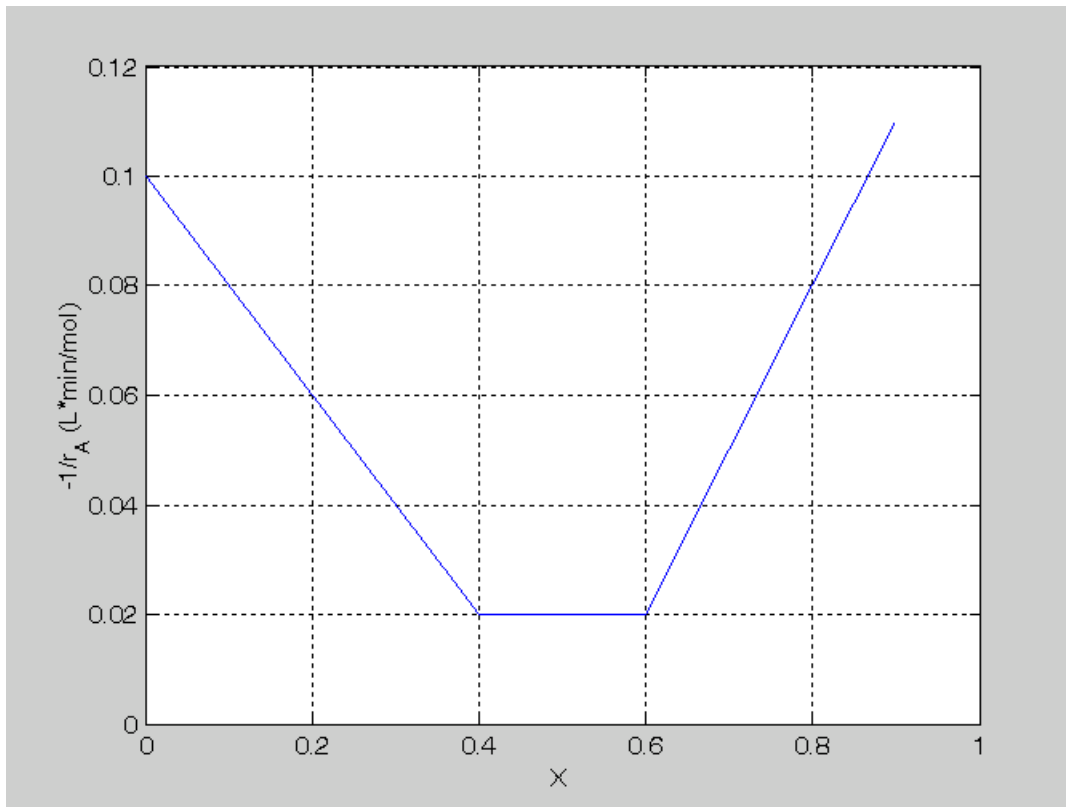


is to be carried out in a flow reactor for an equimolar feed of A and B. What is the value of ε ?

Problem 3e. (10 Points) The exothermic reaction



was carried out adiabatically and the following data are given:



The entering molar flow rate of A was 400 mol/min.

- a. The volume of a CSTR required for 20% conversion is
- b. The volume of a PFR required for 20% conversion is

Numerical Evaluation of Integrals (A.4)

Trapezoidal rule (2-point):

$$\int_0^{X_1} f(x) dx = \frac{h}{2} [f(X_0) + f(X_1)]$$

$$h = X_1 - X_0$$

Simpson's one-third rule (3-point):

$$\int_0^{X_2} f(x) dx = \frac{h}{3} [f(X_0) + 4f(X_1) + f(X_2)]$$

$$h = \frac{X_2 - X_0}{2} \quad X_1 = X_0 + h$$

Simpson's three-eighths rule (4-point):

$$\int_0^{X_3} f(x) dx = \frac{3}{8} h [f(X_0) + 3f(X_1) + 3f(X_2) + f(X_3)] \quad h = \frac{X_3 - X_0}{3}$$

$$X_1 = X_0 + h \quad X_2 = X_0 + 2h$$

Simpson's five-point quadrature :

$$\int_0^{X_4} f(x) dx = \frac{h}{3} [f(X_0) + 4f(X_1) + 2f(X_2) + 4f(X_3) + f(X_4)] \quad h = \frac{X_4 - X_0}{4}$$

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

ABOVE AVERAGE

Above Average Student Original Graded Assignment

Page T4

Kinetics and Reactor Design CHEG 3306 PO 1

Spring 2022

Exam 1 Time: 1Hr 20 min Date: March 9 2022

Instructor: Dr. Nabila Shamim
Total points: 100

ABET OUTCOME 1 An ability to identify, formulate and solve complex engineering problem by applying principle of engineering science and mathematics.

STUDENT NAME: Isaiah Waters DATE: 3/9/2022

Competency area	Points	Score earned
Outcome 1.1 Identify and formulate (i) Understand the given problem and identify the subject area and concepts involved Derive mole balance equation rate law and develop stoichiometry table (ii) Formulate the CEP into a mathematical model [using basic, intermediate and advanced mathematics ranging from algebra & trigonometry, calculus Combine all equation to solve for volume	55	
2.1 Solve problems a. Calculate volume, space time, concentration	45	
Total	100	87

Closed Book Exam NO CELL PHONE USE (PUT THEM AWAY), NO RESTROOM BREAKS NO COLLABORATION
PROVIDE UNITS ON ALL CALCULATIONS AND ANSWERS
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WORK ALL PROBLEMS ON THE QUESTION SHEETS AND DO NOT USE ANY SHEET OF YOUR OWN

Student Signature: Isaiah Waters

Problem 1 (15 points)

The following elementary reaction



$$v_0 = 10 \text{ dm}^3/\text{s}$$

is carried out in a CSTR. For an entering volumetric flowrate of $10 \text{ dm}^3/\text{s}$ at a concentration of 0.5 mol/dm^3 , what is the space time for the reactor to achieve 90% conversion?

$$C_{T0} = 0.5 \text{ mol/dm}^3$$

$$\tau = \frac{V}{v_0}$$

$$X = 0.9$$

Additional Information: $k_A = 0.01 \text{ mol/dm}^3 \cdot \text{s}$

Mole Balance for CSTR

$$V = \frac{F_{A0} X}{-r_A}$$

Rate law:

$$-r_A = k_A C_A C_B^2$$

For CSTR, $v = v_0$

Stoichiometry:

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v_0} = C_{A0}(1-X)$$

$$C_B = \frac{F_B}{v} = \frac{F_{A0}(\theta_B - 2X)}{v_0} = C_{A0}(\theta_B - 2X)$$

$$C_B = 2C_{A0}(1-X)$$

$$C_{T0} = 0.5 \text{ mol/dm}^3 \quad (1/6)$$

$$C_{A0} = 0.5/3 = 0.1667 \text{ mol/dm}^3 \quad (1/3)$$

$$C_{B0} = 0.5(2/3) = 0.333 \text{ mol/dm}^3 \quad (1/3)$$

$$F_{A0} = C_{A0} v_0$$

$$\theta_B = \frac{C_{B0}}{C_{A0}} = \frac{(1/3)}{(1/6)} = 2$$

$$\theta_B = 2$$

$$\frac{\text{mol}}{\text{dm}^3 \cdot \text{s}} \left(\frac{\text{mol}}{\text{dm}^3} \right)^2$$

Combine

$$-r_A = k_A C_{A0}(1-X) [2C_{A0}(1-X)]^2 = 4k_A C_{A0}^3 (1-X)^3$$

$$V = \frac{F_{A0} X}{4k_A C_{A0}^3 (1-X)^3} = \frac{C_{A0} v_0 X}{4k_A C_{A0}^3 (1-X)^3}$$

$$\tau = \frac{V}{v_0} = \frac{X}{4k_A C_{A0}^2 (1-X)^3} = \frac{X}{4(0.01 \text{ mol/dm}^3 \cdot \text{s})(0.1667 \text{ mol/dm}^3)^2 (0.1)^3}$$

$$\tau = 8.1 \times 10^5 \text{ dm}^3/\text{mol}^2 \cdot \text{s}$$

liquid phase
Problem 2 (30 Points) For the gas-phase reaction

Compound A undergoes a reversible isomerization reaction, $A \rightleftharpoons B$, over a supported metal catalyst. Under pertinent conditions, A and B are liquid, miscible, and of nearly identical density; the equilibrium constant for the reaction (in concentration units) is 6.0. In a fixed-bed isothermal flow reactor in which backmixing is negligible (i.e., plug flow), a feed of pure A undergoes a net conversion to B of 50%. The reaction is elementary. If a second, identical flow reactor at the same temperature is placed downstream from the first. The reaction is reversible at constant temperature and pressure.

Follow the CRE algorithms to complete the problem (for example Mole balance equation, Rate laws, Stoichiometry, combine and evaluate etc.)

1. Develop the rate laws
2. Develop the stoichiometric table.
3. Write the concentration of A and B in term of C_{A0} and X .
4. Combine the equations.
5. What overall conversion of A would you expect?

$$K_c = 6.0 \text{ mol/dm}^3$$



Mole Balance

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

1) Rate Laws:

$$-r_A = k_A C_A \quad \leftarrow \text{Forward}$$

$$-r_B = k_B C_B \quad \leftarrow \text{Backward}$$

$$-r_A = k_A C_A - k_B C_B$$

$$= k_A \left(C_A - \frac{k_B}{k_A} C_B \right)$$

$$\frac{k_A}{k_B} = K_c$$

$$\text{net rate} \Rightarrow -r_A = k_A \left(C_A - \frac{C_B}{K_c} \right)$$

2) Stoichiometry

	Initial	Change	Remaining
A	$\frac{F_{A0}}{V_0}$	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	0	$+F_{A0}X$	$F_B = F_{A0}X$

V_0 for liq. phase

At equilibrium, $-r_A = 0$

$$C_A = \frac{C_B}{K_c}$$

$$C_{A0}(1-X) = \frac{C_{A0}X}{K_c}$$

$$3) C_{A1} = \frac{F_A}{V} = \frac{F_{A0}(1-X)}{V_0} = C_{A0}(1-X) \Rightarrow 0.5 C_{A0} \quad \text{50\% conversion}$$

$$C_{B1} = \frac{F_B}{V} = \frac{F_{A0}X}{V_0} = C_{A0}X \Rightarrow 0.5 C_{A0}$$

First reactor

If identical (50% conversion from reactor 1 to 2)

$$C_{A2} = C_{A1}(1-X) = C_{A1}(0.5) = (0.5 C_{A0})(0.5)$$

$$= 0.25 C_{A0}$$

25% conversion

Explain: what would be +2, -2

b) (10 Points) Assuming that the particle diameter is decreased by a factor of 2 so that the pressure drop parameter α , is now increased to 0.02? Assume all other operating conditions are the same as for the base case (i.e. $W = 10$ kg). For a 10 kg PBR with a pressure drop parameter $\alpha = 0.01 \text{ kg}^{-1}$

For the fixed inlet pressure of 10 atm, will the volumetric flow rate v , (dm^3/s), be greater, smaller, or remain the same when the particle diameter is decreased by a factor of 2?

- a. Increased
- ☒ b. Decreased
- c. Remain the same
- d. None of the above

Show your work.

$$v = v_0 (1 + \varepsilon X_A) \left(\frac{Z}{Z_0} \right) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right)$$

$$\frac{dp}{dW} = -\frac{\alpha}{2p} (1 + \varepsilon X)$$

$$p = (1 - \alpha W)^{1/2}$$

$$p = \frac{P}{P_0}$$

$$P_2 = (1 - (0.02)W)^{1/2}$$

increased value

decrease in value

$$P_2 < P_1$$

$$\therefore v = v_0 (1 + \varepsilon X) \underline{p_1}$$

multiplying by a smaller value

V will decrease

Problem 3 (15 Points) The gas phase irreversible reaction is carried out isothermally in a PBR.



The reaction is zero order. The entering temperature is 400 K, and the entering pressure is 10 atm. The flow is turbulent. For a 10 kg PBR with a pressure drop parameter $\alpha = 0.01 \text{ kg}^{-1}$, the exit conversion was found to be 0.4.

a) What catalyst weight of the PBR will you require if you need an exit conversion of 0.8?

$$\frac{dx}{dW} = \frac{-r_A'}{F_{A0}} \quad \checkmark \quad x = 0.8$$

$$-r_A = k_A \quad \checkmark$$

$$P = (1 - \alpha W)^{1/2}$$

$$P = (1 - (0.01)(10))^{1/2} \quad \checkmark$$

$$P = 0.95$$

$$v = v_0 (1 + \epsilon x) P$$

$$W = \frac{F_{A0}}{-r_A} \int dx$$

$$F_{A0} = C_{A0} v_0$$

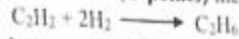
$$W = ?? \quad -2 \text{ catalyst weight}$$

$$P_0 = 10 \text{ atm} \quad P_1 = 0.95(10) = 9.5 \text{ atm}$$

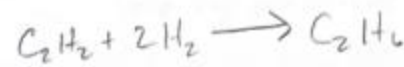
$$\int_{P_0}^{P_1} \frac{dP}{P} = \int_0^W \frac{\alpha}{2(1 + \epsilon x)} dW$$

Handwritten notes in red:
 $\frac{dP}{P} = \frac{\alpha}{2(1 + \epsilon x)} dW$
 $\ln P = \frac{\alpha}{2} \int \frac{dW}{1 + \epsilon x}$

Problem 3c. (5 points) the hydrogenation of acetylene to form ethane



Lets consider 20 Kmole/h acetylene and 50 Kmole/h of hydrogen are fed to the reactor. Which one is the limiting reactant?



20 kmol/h 50 kmol/h

$$\text{C}_2\text{H}_2 \Rightarrow \frac{20 \text{ kmol/h}}{1} = 20$$

$$\text{H}_2 \Rightarrow \frac{50 \text{ kmol/h}}{2} = 25$$

$$\text{C}_2\text{H}_2 \Rightarrow 1(20) = 20$$

$$2\text{H}_2 \Rightarrow 2(25) = 50$$

H₂ is the limiting reactant

Problem 3d. (5 Points) The adiabatic exothermic irreversible gas phase reaction



is to be carried out in a flow reactor for an equimolar feed of A and B. What is the value of ϵ ?

$$C_{A0} = C_{B0}$$

$$\text{A} \Rightarrow (2)(0.5) = 1$$

$$\text{B} \Rightarrow 1(0.5) = 0.5$$

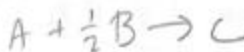
$$\epsilon = y_{A0} \delta$$

$$C_{A0} + C_{B0} = C_T$$

$$\epsilon = 0.5 \left(\frac{2}{2} - \frac{1}{2} - \frac{1}{2} \right)$$

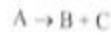
A is limiting

$$\epsilon = -0.25$$

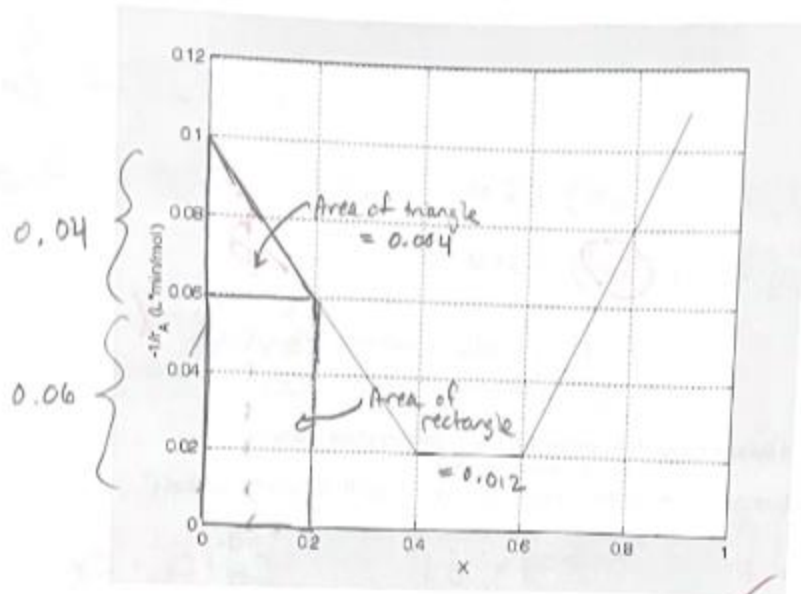


$$\delta = 1 - \frac{1}{2} - 1$$

Problem 3e. (10 Points) The exothermic reaction



was carried out adiabatically and the following data are given:



The entering molar flow rate of A was 400 mol/min.

- a. The volume of a CSTR required for 20% conversion is

$$V = \frac{F_{A0}X}{-r_A} = F_{A0}X \left(\frac{1}{-r_A} \right) \quad @ X = 0.2$$

$$= (400 \text{ mol/min}) (0.2) (0.06 \text{ L·min/mol})$$

$$V = 4.8 \text{ L}$$

- b. The volume of a PFR required for 20% conversion is

Numerical
evaluation
of integrals
not needed
for linear function

$$V = F_{A0} \int \frac{dX}{-r_A}$$

Area under
the curve
rectangle area
triangle area

$$V = (400 \text{ mol/min}) \left[(0.06)(0.2) + \frac{1}{2}(0.04)(0.2) \right]$$

$$V = 6.4 \text{ L}$$

8

AVERAGE

Average Student Original Graded Assignment

Kinetics and Reactor Design CHEG 3306 PO 1

Spring 2022

Exam I Time: 1Hr 20 min Date: March 9 2022

Instructor: Dr. Nabila Shamim

Total points: 100

ABET OUTCOME 1 An ability to identify, formulate and solve complex engineering problem by applying principle of engineering science and mathematics.

STUDENT NAME: Kalya Anderson DATE: 03/09/22

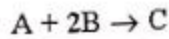
Competency area	Points	Score earned
Outcome 1.1 Identify and formulate (i) Understand the given problem and identify the subject area and concepts involved Derive mole balance equation rate law and develop stoichiometry table (ii) Formulate the CEP into a mathematical model [using basic, intermediate and advanced mathematics ranging from algebra & trigonometry, calculus Combine all equation to solve for volume	55	
2.1 Solve problems a. Calculate volume, space time, concentration	45	
Total	100	65

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Student Signature: Kalya Anderson

Problem 1 (15 points)

The following elementary reaction



is carried out in a CSTR. For an entering volumetric flowrate of $10 \text{ dm}^3/\text{s}$ at a concentration of 0.5 mol/dm^3 , what is the space time for the reactor to achieve 90% conversion?

Additional Information: $k_A = 0.01 \text{ mol/dm}^3 \cdot \text{s}$

$$-r_A = k_A C_A C_B^2, V_0 = 10 \frac{\text{dm}^3}{\text{s}}, k_A = 0.01 \frac{\text{mol}}{\text{dm}^3 \cdot \text{s}}, C_{A0} = 0.5 \frac{\text{mol}}{\text{dm}^3}$$

$$X = 0.9$$

$$V = \frac{F_{A0} X}{-r_A} = V = \frac{C_{A0} V_0 X}{-r_A} \Rightarrow \frac{V}{V_0} = \frac{C_{A0} X}{-r_A} \Rightarrow \tau = \frac{C_{A0} X}{-r_A}$$

Species	in	change	remaining
A	C_{A0}	$-C_{A0} X$	$C_A = C_{A0} (1-X)$
B	$C_{B0} = \theta_B C_{A0}$	$-2C_{A0} X$	$C_B = C_{A0} (\theta_B - 2X)$
C	—	$+C_{A0} X$	$C_C = C_{A0} X$

$$\theta_B = \frac{C_{B0}}{C_{A0}} = ?$$

$$-r_A = k_A C_A C_B^2 = (0.01 \frac{\text{mol}}{\text{dm}^3 \cdot \text{s}}) (C_{A0} (1-X)) (C_{A0} (\theta_B - 2X))^2$$

$$= 0.01 (C_{A0})^2 (1-X) (\theta_B - 2X)^2$$

$$\tau = \frac{C_{A0} X}{0.01 (C_{A0})^2 (1-X) (\theta_B - 2X)^2} = \frac{1 (0.9)}{(0.01 \frac{\text{mol}}{\text{dm}^3 \cdot \text{s}}) (C_{A0} X (1-X) (\theta_B - 2X)^2)}$$

$$\tau = \frac{1 (0.9)}{(0.01 \frac{\text{mol}}{\text{dm}^3 \cdot \text{s}}) (0.5 \frac{\text{mol}}{\text{dm}^3}) (1-0.9) (\theta_B - 2(0.9))} = \frac{0.9}{0.005 (1-0.9) (\theta_B - 1.8)}$$

Kalaya Anderson

Problem 3 (15 Points) The gas phase irreversible reaction is carried out isothermally in a PBR.



The reaction is zero order. The entering temperature is 400 K, and the entering pressure is 10 atm. The flow is turbulent. For a 10 kg PBR with a pressure drop parameter $\alpha = 0.01 \text{ kg}^{-1}$, the exit conversion was found to be 0.4.

a) What catalyst weight of the PBR will you require if you need an exit conversion of 0.8?

Given Info:

zero order $= -r_A' = k$, $T = 400 \text{ K}$, $P = 10 \text{ atm}$, $X = 0.8$

"gas phase isothermal rxn" $= T = T_0$, $\epsilon = 0$

$$v = v_0(1 + \epsilon X) \frac{T}{T_0} \frac{P_0}{P} \Rightarrow v = v_0(1) \quad P = v = v_0 P$$

1) Mole Balance: $F_{A0} \frac{dX}{dW} = -r_A'$

2) Rate Law: $-r_A' = k_A$

3) Stoichiometry

Species	In	Change	Remaining
A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	0	$+F_{A0}X$	$F_B = F_{A0}X$

4) $\frac{dX}{dW} = \frac{k_A}{F_{A0}}$

$$\int_0^{10} dW = \frac{F_{A0}}{k_A} \int_0^{0.4} dX \Rightarrow (10-0) = \frac{F_{A0}}{k_A} (0.4-0) \Rightarrow 10 k_A = F_{A0} (0.4)$$

$$F_{A0} = 25 k_A$$

5) $\frac{dX}{dW} = \frac{k_A}{F_{A0}} \Rightarrow \int_0^{0.8} dW = \frac{F_{A0}}{k_A} \int_0^{0.8} dX \Rightarrow W = \frac{25 k_A}{k_A} (0.8-0)$

$$W = 25(0.8-0) = \boxed{W = 20 \text{ kg}}$$

For the fixed inlet pressure of 10 atm, will the volumetric flow rate v , (dm^3/s), be greater, smaller, or remain the same when the particle diameter is decreased by a factor of 2?

- a. Increased
b. Decreased
c. Remain the same
d. None of the above

assuming isothermal so $T=T_0$ and $\epsilon=0$

Show your work.

Show your work.

$$v = v_0 (1 - \varepsilon X_A) \left(\frac{Z}{Z_0} \right) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right) \Rightarrow v = v_0 \frac{1}{\gamma \rho}$$

$$\frac{dp}{dW} = -\frac{\alpha}{2p}(1+\varepsilon_X) \quad \underline{p = (1 - \alpha W)^{1/2}}$$

$$\underline{V = V_0 \left(\frac{1}{p} \right)}$$

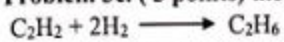
$$\underline{V = V_0 \left(\frac{1}{p} \right)}$$

For $a = 0.01 \frac{1}{\text{kg}}$; $p = (1 - (0.01 \frac{1}{\text{kg}})(10 \text{ kg}))^{1/2} = p_1 = 0.948$ $\frac{1}{p_1} = 1.05$

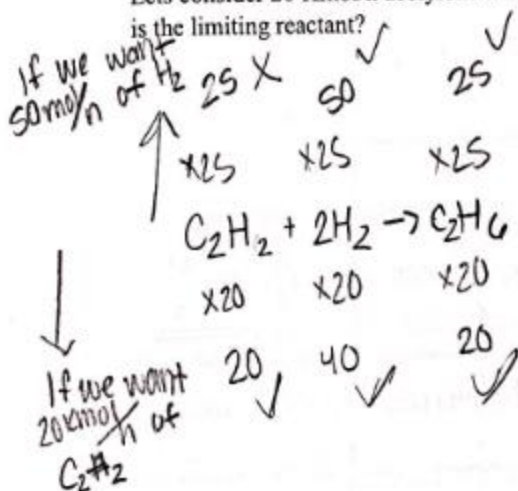
For $a = 0.02 \frac{1}{\text{kg}}$; $p = (1 - (0.02 \frac{1}{\text{kg}})(20 \text{ kg}))^{1/2} = p_2 = 0.775 \frac{1}{p_2} = 1.29$

Applying p to $v = v_0(\frac{1}{p})$, v and $(\frac{1}{p})$ are directly related. Keep in mind that $p = \frac{P}{P_0}$ so we took the inverse to be able to plug it in the v equation. So from $\frac{1}{p_1}$ to $\frac{1}{p_2}$, applying it to the eq. will show that v will increase as we decrease the alpha (α) value.

Problem 3c. (5 points) the hydrogenation of acetylene to form ethane

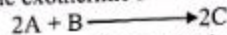


Lets consider 20 Kmol/h acetylene and 50 Kmol/h of hydrogen are fed to the reactor. Which one is the limiting reactant?



C_2H_2 is the limiting reactant.

Problem 3d. (5 Points) The adiabatic exothermic irreversible gas phase reaction



is to be carried out in a flow reactor for an equimolar feed of A and B. What is the value of ϵ ?

$\epsilon = y_{A0} \delta$, equimolar $\Rightarrow y_{A0} = 0.50$

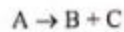
$\delta = \frac{2 - 2 - 1}{-1} = -1$ reactant

$\epsilon = (0.50)(-1)$

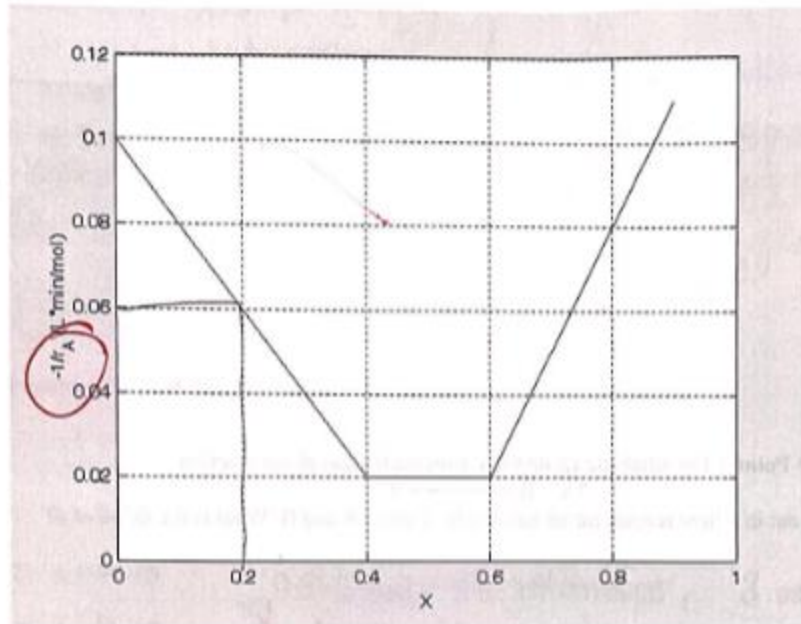
$\epsilon = -1$

which one is limiting -2

Problem 3c. (10 Points) The exothermic reaction



was carried out adiabatically and the following data are given:



The entering molar flow rate of A was 400 mol/min.

a. The volume of a CSTR required for 20% conversion is

$$V_{CSTR} = \frac{F_{A0} X}{-r_{A,exit}} = \frac{400 \frac{\text{mol}}{\text{min}}}{0.06 \frac{\text{mol}}{\text{min} \cdot \text{L}}} (0.20) = V_{CSTR} = 1333.3 \text{ L}$$

b. The volume of a PFR required for 20% conversion is

$$V = \int_0^X \frac{F_{A0}}{-r_A} dX \quad ; \text{ using 2-pt. rule}$$

$$\eta = X_1 - X_0 = 0.2 - 0 = 0.2$$

$$\int_0^{X_1} f(x) dx = \frac{\eta}{2} (f(x_0) + f(x_1)) \quad , \quad f(x_0) = \frac{F_{A0}}{-r_{A, X_0}} = \frac{400}{0.1} = 4000 \text{ L}$$

$$f(x_1) = \frac{F_{A0}}{-r_{A, X_1}} = \frac{400}{0.06} = 6666.67 \text{ L}$$

$$= \frac{0.2}{2} (4000 \text{ L} + 6666.67 \text{ L})$$

$$V_{PFR} = 1066.67 \text{ L}$$

BELOW AVERAGE

Below Average Student Original Graded Assignment

Kinetics and Reactor Design CHEG 3306 PO 1

Spring 2022

Exam I Time: 11hr 20 min Date: March 9 2022

Instructor: Dr. Nabila Shamim
Total points: 100

ABET OUTCOME 1 An ability to identify, formulate and solve complex engineering problem by applying principle of engineering science and mathematics.

STUDENT NAME: Yasmine Ramez.....DATE: March 9.....

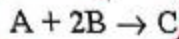
Competency area	Points	Score earned
Outcome 1.1 Identify and formulate (i) Understand the given problem and identify the subject area and concepts involved Derive mole balance equation rate law and develop stoichiometry table (ii) Formulate the CEP into a mathematical model [using basic, intermediate and advanced mathematics ranging from algebra & trigonometry, calculus Combine all equation to solve for volume	55	
2.1 Solve problems a. Calculate volume, space time, concentration	45	
Total	100	41

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WORK ALL PROBLEMS ON THE QUESTION SHEETS AND DO NOT USE ANY SHEET OF YOUR OWN

Student Signature: 

Problem 1 (15 points)

The following elementary reaction



is carried out in a CSTR. For an entering volumetric flowrate of $10 \text{ dm}^3/\text{s}$ at a concentration of 0.5 mol/dm^3 , what is the space time for the reactor to achieve 90% conversion?

Additional Information: $k_A = 0.01 \text{ mol/dm}^3 \cdot \text{s}$

$$V_{\text{CSTR}} = \frac{F_{A0}}{-r_A} (X_A)$$

$$X_A = 90\% = 0.9$$

$$C_{A0} = 0.5 \text{ mol/dm}^3$$

$$V = 10 \text{ dm}^3/\text{s}$$

$$K = 0.01 \text{ mol/dm}^3 \cdot \text{s}$$

$$-r_A = K C_A C_B^2$$

45 sec

$$\frac{\tau}{C_{A0}} = \frac{X_A}{-r_A}$$

rate law?
-10

$$\frac{\frac{\text{mol}}{\text{dm}^3} \cdot \frac{\text{dm}^3}{\text{mol}}}{\frac{\text{mol}}{\text{dm}^3 \cdot \text{s}}} = \frac{1}{\text{s}}$$

$$\tau = \frac{X_A (C_{A0})}{-r_A} = \frac{(0.9)(0.5 \text{ mol/dm}^3)}{(0.01 \frac{\text{mol}}{\text{dm}^3 \cdot \text{s}})}$$

2

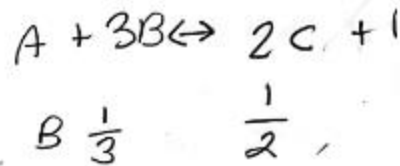
Problem 3 (30 Points)

Problem 3a. (5 Points) Given the following liquid phase reaction and feed conditions what is the correct expression for C_D as a function of the conversion of the limiting reactant X ?

$$A + 3B \rightleftharpoons 2C + D$$

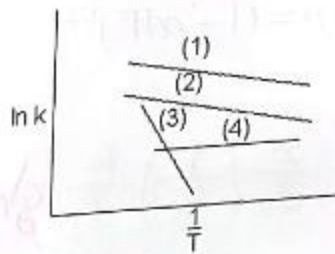
$$C_{A0} = C_{D0} = 1 \text{ mol/min} \quad C_{B0} = 2 \text{ mol/min} \quad C_{C0} = 0$$

- a) $C_D = C_{B0} (1-X)$
- b) $C_D = C_{B0} (1+X)$
- c) $C_D = C_{B0} (1-X/3)$
- d) $C_D = C_{B0} (1/2 + X/3)$**



Problem 3b. (5 Points) Consider the following elementary reactions

- 1) $A \xrightarrow{k_1} B$
- 2) $A \xrightarrow{k_2} D$
- 3) $A \xrightarrow{k_3} Y$
- 4) $A \xrightarrow{k_4} U$



Slope

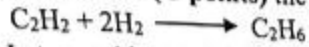
a) Which reaction has the higher activation energy?

3

b) Which reaction is virtually temperature insensitive?

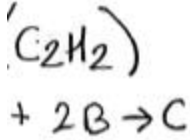
4

Problem 3c. (5 points) the hydrogenation of acetylene to form ethane



Lets consider 20 Kmol/h acetylene and 50 Kmol/h of hydrogen are fed to the reactor. Which one is the limiting reactant?

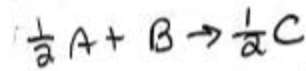
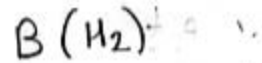
$$\begin{aligned}\text{C}_2\text{H}_2 &= 20 \text{ Kmol/h} & \text{A} \\ 2\text{H}_2 &= 50 \text{ Kmol/h} & \text{B}\end{aligned}$$



$$1) = 20 \text{ moles A}$$

$$2) = 40 \text{ moles B}$$

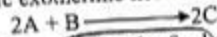
∴ limiting reactant is C_2H_2



$$\frac{1}{2}(50) = 25 \text{ moles A}$$

$$1(50) = 50 \text{ moles B}$$

Problem 3d. (5 Points) The adiabatic exothermic irreversible gas phase reaction

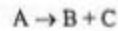


is to be carried out in a flow reactor for an equimolar feed of A and B. What is the value of ϵ ?

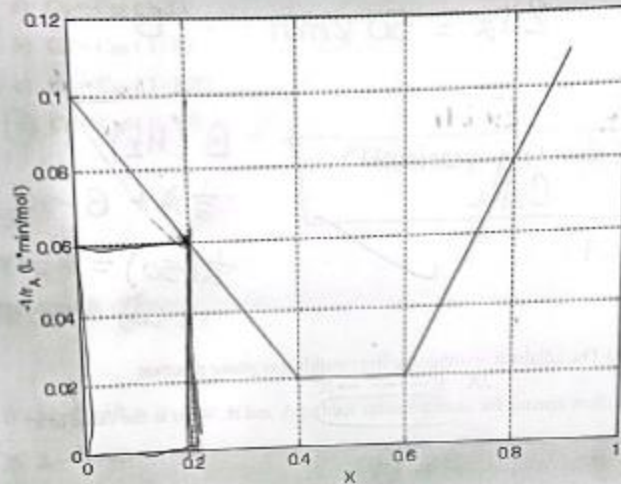
$$\text{A} = \text{B}$$

-5

Problem 3e. (10 Points) The exothermic reaction



was carried out adiabatically and the following data are given:



$$F_{A0} = 400 \frac{\text{mol}}{\text{min}}$$

$$\frac{400}{0.1} = 4000$$

The entering molar flow rate of A was 400 mol/min.

The volume of a CSTR required for 20% conversion is

$$\frac{400}{0.06} = 6666$$

a.

$$(0.2)(0.06) = 0.012 \text{ dm}^3 = 0.012 \text{ L}$$

b.

The volume of a PFR required for 20% conversion is

$$\int_0^{0.2} \frac{F_{A0}}{-r_A} dx$$

$$\int_0^{0.2} \frac{r_{A0}}{-r_A} dx = \frac{0.2}{2} [4000 + 6666]$$

$$V = 1066$$

Two Point rule

$$\int_0^{0.2} \frac{F_{A0}}{-r_A} = \frac{h}{2} [f(x_0) + f(x_1)]$$

$$h = x_1 - x_0$$

$$h = 0.2 - 0 = 0.2$$

CHEG 3306-P01: KINETICS AND REACTOR DESIGN

Title of Assignment: Quiz 1

TOPICS COVERED IN Quiz 1

Quiz 1 covered the following topics:

Mole Balance, Stoichiometry

CHEG 3306-P01: KINETICS AND REACTOR DESIGN

**SAMPLE TEST QUESTIONS, SOLUTION,
AND GRADING SCHEME FOR Quiz**

Above AVERAGE

Name: Isaiah Waters

20

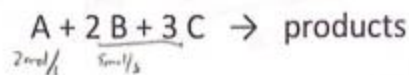
Chemical Reaction Engineering CHEG 3306

Quiz 1 (25 Points) January 26 2022

Mole Balance

Problem 1 (5 Points each)

- 1) For the reaction below, which is the limiting reactant?



$$F_{A0} = 2 \text{ mol/sec}, F_{B0} = F_{C0} = 5 \text{ mol/sec}$$

$$A \Rightarrow 2 \text{ mol/s}$$

$$2B \Rightarrow 5 \text{ mol/s} \Rightarrow 2.5 \text{ mol/s}$$

$$3C \Rightarrow 5 \text{ mol/s} \Rightarrow 1.67 \text{ mol/s}$$

A) A

B) B

C) C

- 2) Which change cannot increase the rate $-r_A$?

~~A) Raise temperature~~

B) Use better catalyst

C) Switch to better type reactor

D) Change solvent in liquid phase reaction

3) Which information below is used in deriving the design equation for a batch reactor?

Answer choices

a) $G_j = V \cdot R_j$

b) $f_{j0} = F_j = 0$

c) $dN_j/dt = 0$

d) $E = mc^2$

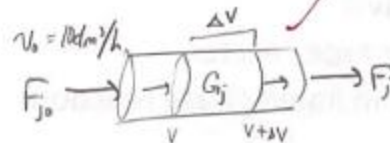
Problem 2 (10 Points) The first order reaction $A \rightarrow B$ is carried out in a tubular reactor in which the volumetric flow rate v_0 is constant.

Packed Flow
Reactor

- Derive an equation relating the reactor volume to the entering and exiting concentration of A, the rate constant K and the volumetric flow rate v_0 .
- Determine the reactor volume necessary to reduce the existing concentration to 1% of the entering concentration when the volumetric flow rate is $10 \text{ dm}^3/\text{min}$ and the specific reaction rate k is 0.23 /min

Grading Method

- Understand the given problem and identify the subject area and concepts involved. Convert the problem into a well labeled sketch.
- Formulate the problem into a mathematical model stating all relevant assumptions.
- Solve the resulting mathematical formulations numerically.



Tubular / PFR

Steady-state

Radial distribution constant

a.) GMBE

$$F_{j0} - F_j + G_j = \frac{dN_j}{dt} \rightarrow F_j|_V - F_j|_{V+\Delta V} + \int_V^{V+\Delta V} r_j dV = 0$$

cont...

Name:

$$F_j|_V - F_j|_{V+\Delta V} + r_j \Delta V = 0$$

$$r_j \Delta V = F_j|_{V+\Delta V} - F_j|_V$$

$$r_j = \frac{F_j|_{V+\Delta V} - F_j|_V}{\Delta V}$$

$$\lim_{\Delta V \rightarrow 0} \frac{F_j|_{V+\Delta V} - F_j|_V}{\Delta V}$$

$$r_j = \frac{dF_j}{dV}$$

In terms of A ...

$$r_A = \frac{dF_A}{dV}$$

$$\int_0^V dV = \int_{F_{A_0}}^{F_A} \frac{dF_A}{r_A}$$

$$V = \frac{F_A - F_{A_0}}{r_A} = \frac{F_{A_0} - F_A}{-r_A} = KC_A$$

$$F_A = V_0 C_A$$

$$V = \frac{F_{A_0} - F_A}{KC_A} \Rightarrow \frac{V_0 C_{A_0} - V_0 C_A}{KC_A}$$

$$a) \boxed{V = \frac{V_0 (C_{A_0} - C_A)}{KC_A}}$$

3

b.)

$$V = \frac{V_0 (C_{A0} - C_A)}{k C_A}$$

$$k = 0.23/\text{min}$$

$$V_0 = 10 \text{ dm}^3/\text{min}$$

$$C_A = 0.01 C_{A0}$$

$\Downarrow$

$$100 C_A = C_{A0}$$

$$V = \frac{V_0 (100 C_A - C_A)}{k C_A}$$

$$V = \frac{V_0 (99 C_A)}{k C_A}$$

$$V = \frac{99 V_0}{k} = \frac{99 (10 \text{ dm}^3/\text{min})}{(0.23/\text{min})}$$

$$\boxed{V = 4304 \text{ dm}^3}$$

AVERAGE

Name: *Oluwatunmbi Alade*

12

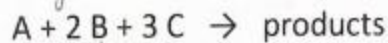
Chemical Reaction Engineering CHEG 3306

Quiz 1 (25 Points) January 26 2022

Mole Balance

Problem 1 (5 Points each)

- 1) For the reaction below, which is the limiting reactant? *limiting reactant: reactant that produces less*



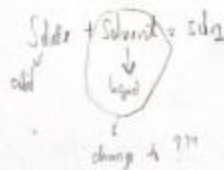
$F_{A0} = 2 \text{ mol/sec}, F_{B0} = F_{C0} = 5 \text{ mol/sec}$

- 5*
☒ A) A
☐ B) B
☐ C) C

- 2) Which change cannot increase the rate $-r_A$?

A → B disappearance of A

- 5*
A) Raise temperature ↑
B) Use better catalyst ↑
C) Switch to better type reactor
D) Change solvent in liquid phase reaction *solubility?*



Name: Oluwatunmbi Alade.

3) Which information below is used in deriving the design equation for a batch reactor?

Answer choices

a) $G_j = V \cdot R_j$

☒ b) $F_{j0} = F_j = 0$

c) $dN_j/dt = 0$

d) $E = mc^2$

For batch: $\dot{N}_j^0 - \dot{N}_j^0 + G_{jn} = \text{Accu}$
 $F_{j0} - F_j + \int r_n dV = \frac{dN_j}{dt}$
 $dt = \frac{1}{r_n} \int dN_j$

Problem 2 (10 Points) The first order reaction $A \rightarrow B$ is carried out in a tubular reactor in which the volumetric flow rate v_0 is constant.

PFR tubes

$V, V_0 = 10 \text{ dm}^3/\text{hr}$

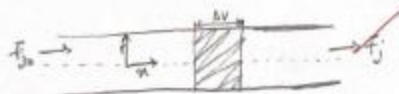
$f = V \cdot C$

$C_{A0}, V, k, V_0,$

- Derive an equation relating the reactor volume to the entering and exiting concentration of A, the rate constant K and the volumetric flow rate v_0 .
- Determine the reactor volume necessary to reduce the existing concentration to 1% of the entering concentration when the volumetric flow rate is $10 \text{ dm}^3/\text{min}$ and the specific reaction rate k is 0.23 /min

Grading Method

- Understand the given problem and identify the subject area and concepts involved. Convert the problem into a well labeled sketch.
- Formulate the problem into a mathematical model stating all relevant assumptions.
- Solve the resulting mathematical formulations numerically.



$\dot{N}_j^0 - \dot{N}_j^0 + G_{jn} = \text{Accu}$

$F_{j0} - F_j + \int r_n dV = \frac{dN_j}{dt}$

$F_{j0} - F_{j0+dv} = -\int r_n dV$

$\int r_n = \frac{F_{j0} - F_{j0+dv}}{dv}$

Taking Limit of both sides

$r_n = \frac{dF_n}{dV}$

Assuming:
 Steady state
 Packed flow reactor because of tubes
 1st order reaction ($-r_n = K C_A$)

Name: Dhuwatuminou Alade

$$K = 0.23/\text{min}$$

$$V_0 = 10 \text{ dm}^3/\text{min}$$

$$r_A = \frac{dF_A}{dV} \quad \checkmark$$

$$r_A = C_A V_A$$

$$-r_A = V_A \cdot \frac{dC_A}{dV}$$

$$C_A = 0.01 C_{A0}$$

$$-r_A = K C_A$$

$$-r_A = K \times 0.01 C_{A0}$$

$$-r_A = 0.23 \times 0.01 C_{A0}$$

$$-r_A = 0.0023 C_{A0}$$

$$V_0 = 10$$

$$\text{So, } 0.0023 C_{A0} = \frac{V_A \times 0.01 C_{A0}}{(10)}$$

$$V_A = \frac{0.0023 \times 10}{0.01} \quad \checkmark$$

$$V_A = \underline{\underline{2.3 \text{ dm}^3}}$$

Below AVERAGE

Name: Yazmine Rincon

7

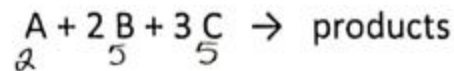
Chemical Reaction Engineering CHEG 3306

Quiz 1 (25 Points) January 26 2022

Mole Balance

Problem 1 (5 Points each)

- 1) For the reaction below, which is the limiting reactant?



$$F_{A0} = 2 \text{ mol/sec}, F_{B0} = F_{C0} = 5 \text{ mol/sec}$$

- ~~A) A~~
B) B
C) C

5

- 2) Which change cannot increase the rate $-r_A$?

- ~~5~~
A) Raise temperature
~~B) Use better catalyst~~
C) Switch to better type reactor
D) Change solvent in liquid phase reaction

Name:

3) Which information below is used in deriving the design equation for a batch reactor?

Answer choices

a) $G_j = V \cdot R_j$

b) $F_{j0} = F_j = 0$

c) $dN_j/dt = 0$

d) $E = mc^2$

Problem 2 (10 Points) The first order reaction $A \longrightarrow B$ is carried out in a tubular reactor in which the volumetric flow rate v_0 is constant.

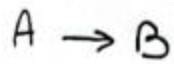
- Derive an equation relating the reactor volume to the entering and exiting concentration of A, the rate constant K and the volumetric flow rate v_0 .
- Determine the reactor volume necessary to reduce the existing concentration to 1% of the entering concentration when the volumetric flow rate is $10 \text{ dm}^3/\text{min}$ and the specific reaction rate k is 0.23 /min

$$-r_A = kC_A \quad v_0 = 10 \frac{\text{dm}^3}{\text{hr}}$$

Grading Method

- Understand the given problem and identify the subject area and concepts involved. Convert the problem into a well labeled sketch.
- Formulate the problem into a mathematical model stating all relevant assumptions.
- Solve the resulting mathematical formulations numerically.

Name:



Tubular reaction

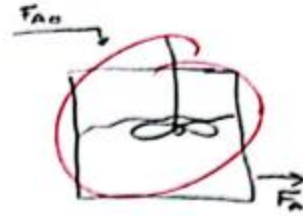
Knowns

$$-r_A = kC_A$$

$$V_0 = 10 \frac{\text{dm}^3}{\text{min}}$$

Tubular reaction

$$\frac{F_{A0} - F_A}{-r_A} = V \quad \text{CSTR}$$



tubular

60

Steady State
Spatial Variation?
Perfectly mixed?

$$\frac{F_{A0} - F_A}{kC_A} = V = \underline{\underline{0.23}}$$

**CHEMICAL ENGINEERING DEPARTMENT
KINETICS AND REACTOR DESIGN CHEG 3306 P01
SPRING 2022**

Assignment 3

TOPICS COVERED

- 1. Formulate and Solve Reaction Engineering Problem (multiple Reaction) using POLYMATH/MATLAB**

**CHEMICAL ENGINEERING DEPARTMENT
KINETICS AND REACTOR DESIGN CHEG 3063 Y01
SPRING 2022**

**Assignment #3 QUESTIONS, SOLUTION,
AND GRADING SCHEME**

Chemical Reaction Kinetics and Reactor Design CHEG 3306 PO 1 (Spring 2022):
Assignment 3 Due Date: April 18, 2022

STUDENT NAME:DATE:

Open Book Assignment

Upload the graded homework in task stream under Outcome1Multiple Reactions (use Polymath)

Student Signature:

Chemical Reaction Engineering CHEG 3306

SPRING 2022

Homework Assignment 3: DUE DATE April 18 2022

Chapter 6: Isothermal Reactor Design: Moles and Molar flow rates

Text Book: Elements of Chemical Reaction Engineering, 6TH Edition, by H. Scott Fogler

Problems:

Problem P6 -4_B, Problem P6-7_B and Problem 6-11_B

P6-4 Problem Statement:

The elementary gas-phase reaction

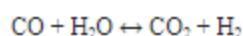
Is carried out isothermally at 400 K in a flow reactor with no pressure drop. The specific reaction rate at 50°C is 10 min (from pericosity data) and the activation energy is 85 kJ/mol. Pure di-tert-butyl peroxide enters the reactor at 10atm and 127°C and a molar flow rate of 2.5mol/min, that is, $F = 2.5\text{mol/min}$.



1. Use the algorithm for molar flow rates to formulate and solve the problem. Plot F_A , F_B , F_C , and then X as a function of plug-flow reactor volume and space time to achieve 90% conversion.
2. Calculate the plug-flow volume and space time for a CSTR for 90% conversion

Problem P6-7_B Problem Statement

Fuel Cells Rationale. With the focus on alternative clean-energy sources, we are moving toward an increased use of fuel cells to operate appliances ranging from computers to automobiles. For example, the hydrogen/oxygen fuel cell produces clean energy as the products are water and electricity, which may lead to a hydrogen-based economy instead of a petroleum-based economy. A large component in the processing train for fuel cells is the water-gas shift membrane reactor. (M. Gummala, N. Gupta, B. Olsomer, and Z. Dardas, Paper 103c, 2003, AIChE National Meeting, New Orleans, LA.)



Here, CO and water are fed to the membrane reactor containing the catalyst. Hydrogen can diffuse out the sides of the membrane, while CO, H₂O, and CO₂ cannot. Based on the following information, plot the concentrations and molar flow rates of each of the reacting species down the length of the membrane reactor. Assume the following: The volumetric feed is 10 dm³/min at 10atm, and the equimolar feed of CO and water vapor with C_{T0} = 0.4mol/dm³. The equilibrium constant is K_e = 1.44, with k = 1.37 dm⁶/mol kg-cat · min, and the mass transfer coefficient k_{H₂} = 0.1 dm³/kg-cat · min (Hint: First calculate the entering molar flow rate of CO and then relate F_A and X.)

- (a) What is the membrane reactor volume necessary to achieve 85% conversion of CO?
- (b) Sophia wants you to compare the MR with a conventional PFR. What will you tell her?
- (c) For that same membrane reactor volume, Nicolas wants to know what would be the conversion of CO if the feed rate were doubled?

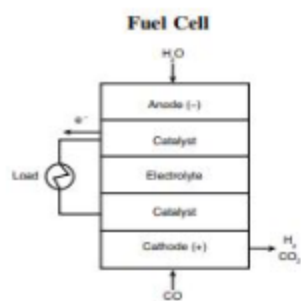


Fig. 6

Problem 4-11₈ Problem Statement

Pure butanol is to be fed into a semibatch reactor containing pure ethyl acetate to produce butyl acetate and ethanol. The reaction



is elementary and reversible. The reaction is carried out isothermally at 300 K. At this temperature, the equilibrium constant is 1.08 and the specific reaction rate is $9 \times 10^{-5} \text{ dm}^3/\text{mol} \cdot \text{s}$. Initially, there is 200 dm³ of ethyl acetate in the vat, and butanol is fed at a volumetric rate of 0.05 dm³/s. The feed and initial concentrations of butanol and ethyl acetate are 10.93 mol/dm³ and 7.72 mol/dm³, respectively.

- (a) Plot and analyze the equilibrium conversion of ethyl acetate as a function of time.
- (b) Plot and analyze the conversion of ethyl acetate, the rate of reaction, and the concentration of butanol as a function of time.

ABOVE AVERAGE

Above Average Student Original Graded Assignment

Prairie View A&M University
Roy G. Perry College of Engineering
Department: Chemical Engineering



CHEG 3063 – P01
Chemical Reaction Kinetics and Reactor Design
Project:
Polymath Assignment #1
Date Due: Friday March 11, 2021

Submitted by: Kennedy Dent

Submitted to: Dr. Nabila Shamim

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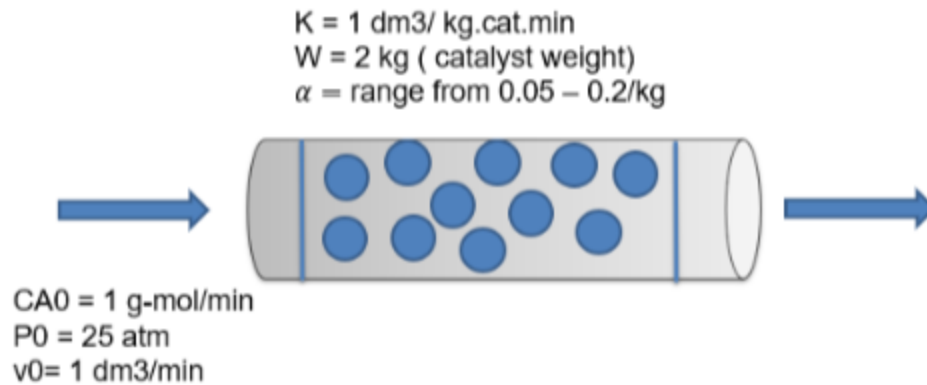
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Problem Statement 1:

The catalytic gas phase reaction $A \rightarrow B$ is to be carried out in a packed bed reactor under isothermal operation. The reactant is pure A with an inlet concentration of 1 g-mol/dm³, the entering pressure is 25 atm and the entering volumetric flow rate is 1 dm³/min. the first order reaction rate constant K, which is based on reactant A is 1 dm³/kg.cat. min.

1. Develop the chemical reaction engineering algorithm, - mole balance, rate laws stoichiometry and combine them together, finally solve the following using Polymath/MATLAB.
2. Study the effect of the pressure drop on the conversion for the first order reaction and plot conversion and pressure ($p = P/P_0$) as a function of the weight of the packing material W. consider the pressure drop parameter α is between 0.05 – 0.2 /kg. also consider the maximum weight of the catalyst is 2 kg.

Schematic Diagram



Assumptions

To successfully evaluate the Packed bed reactor, we must assume the following.

- The process is isothermal ($T=T_0$)
- Flow is due to gravity

- There is a reaction occurring at the surface of the catalysts
- Elementary Gas Phase Reaction

Identify

The identify, formulate, and solve methodology is a tool used to carefully analyze engineering problems. The identify step will list the given information. The problem statements lists the following parameters

Given Information:

CA_0 (Initial Concentration of species A) = 1 g-mol/ dm³

v_0 (Initial Volumetric Flow Rate) = 1 dm³ /min

P_0 (Initial Pressure) = 25 atm

K (Rate Constant) = 1 dm³ / kg.cat. min

α = ranges from (0.05-0.2)/kg

W (catalyst weight) = 2 kg

Formulate

The formulate step consists of preparing equations and steps needed to complete a project. The following equations and information allowed us to carefully analyze the packed bed reactor.

Mole Balance

For a packed bed reactor (PBR),

$$\frac{dX_A}{dW} = \frac{r'_A}{F_{A0}}$$

The mole balance for the packed bed reactor includes the differential value, X_A , which represents the conversion factor of species A entering the reactor. The variable W represents the Weight of the catalyst, F_{A0} is the Initial Molar flow rate of species A, and r'_A is the rate law and is dependent on the concentration of a species.

Rate Law

$$r'_A = k C_{A0}$$

The rate Law equation developed from the reaction given in the problem statement will assist in calculating the weight of the catalyst.

Stoichiometric Table

Table 1: Problem 1 Stoichiometric Table

Symbol	Initial	Change	Remaining	Concentration
A	C_{A0}	$-C_{A0}X_A$	$C_{A0} - C_{A0}X_A$	$C_A = C_{A0} \frac{1 - X_A}{1 + \varepsilon X_A} * \frac{P}{P_0}$
B	0	$+C_{A0} X_A$	$0 + C_{A0}X_A$	$C_B = C_{A0} \frac{X_A}{1 + \varepsilon X_A} * \frac{P}{P_0}$

In the table above species, A and B are analyzed. C_A and C_B are the concentrations of both A and B and include the conversion X_A . ε represents the product of delta and the mole fraction of A in the gas phase. Delta is the sum of stoichiometric coefficients of the reactants and products. This table also includes the expression P/P_0 which represents the pressure drop in the reactor. The denominator of the C_A and C_B equations was added to account for the gas phase reaction. The equation below substitutes the rate law into the packed bed mole balance equation.

$$\frac{dX_A}{dW} = k * C_{A0} \frac{1 - X_A}{1 + \varepsilon X_A} * \frac{P}{P_0} \frac{1}{F_{A0}}$$

Where $k * C_{A0} \frac{1 - X_A}{1 + \varepsilon X_A} * \frac{P}{P_0}$ is the rate law equation under isothermal conditions with pressure drop.

Polymath Program Results

```
Differential Equations: 2 Auxiliary Equations: 12 ☒ Ready for solution

# Kinetics Homework 2
# Kennedy Dent
# Dr. Nabila Shamim
# Problem 1

FA0 = CA0 * v0
CA0 = 1 # Initial Molar Flow rate (g-mol/dm^3)
v0 = 1 # Initial Volumetric Flow rate (dm^3/min)
rA = (k * CA0 * (1 - XA) * y)
d(XA)/d(W) = rA / FA0 # Mole Balance Equation for Packed Bed Reactor
W(0) = 0
W(f) = 2 # Maximum weight of the Catalyst (kg)
XA(0) = 0
eps = yA0 * delta
delta = 0
yA0 = 1
d(p)/d(W) = -alpha * (1 + eps * XA / 2 * y) # Differential form of Ergun's Equation
y = (1 - alpha * W) ^ 0.5
P0 = 25 # Pressure (atm)
alpha = (0.05 + 0.2) / 2 # Alpha
k = 1 # Rate Constant (dm^3/kg cat min)
p(0) = 1
P = P0 * (1 - alpha * W) ^ 0.5 # Final Pressure (atm)
```

Figure 1: Polymath Algorithm

The Polymath application allowed me to input the algorithms, equations, and initial values to solve key parameters for the packed bed reactor. All variables were clearly defined in the application and the Ergun's equation was used to relate pressure drop and the catalyst weight. The alpha term was found by taking the average of the range of (0.05 – 0.2).

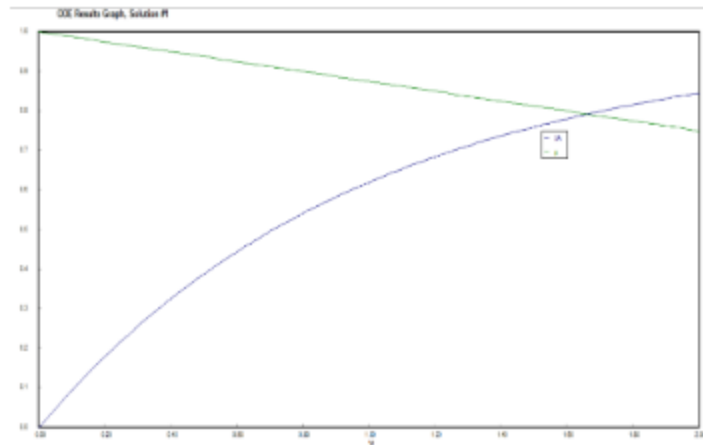


Figure 2: Packed Bed Reactor with Pressure Drop (Conversion vs catalyst weight)

Figure 2 above is a graph generated by Polymath that show the effects of pressure on conversion. Again, we can observe that the pressure drop causes a decrease in the conversion of our reactor. The x-axis represents the weight of the catalyst and the y-axis.

Solve

Solving is the final step in the three-step methodology. In this step, we use the equations we derived and manipulated to find the values needed. The Polymath algorithm solved the missing parameters as shown below.

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	W	0	0	2.	2.
2	XA	0	0	0.8457579	0.8457579
3	p	1.	0.75	1.	0.75
4	v0	1.	1.	1.	1.
5	CA0	1.	1.	1.	1.
6	FA0	1.	1.	1.	1.
7	k	1.	1.	1.	1.
8	yA0	1.	1.	1.	1.
9	delta	0	0	0	0
10	eps	0	0	0	0
11	alpha	0.125	0.125	0.125	0.125
12	P0	25.	25.	25.	25.
13	y	1.	0.8660254	1.	0.8660254
14	rA	1.	0.1335776	1.	0.1335776
15	P	25.	21.65064	25.	21.65064

Figure 3: Generated values for the packed bed reactor using the Polymath Algorithm

Figure 3 above displays the parameters generated by the Polymath Algorithm. The final pressure was 21.65 atm and the final conversion value of A was 0.85.

Conclusion:

In conclusion, the Polymath algorithm allowed us to successfully solve the conversion and study the effect of pressure drop on the conversion. By developing the engineering algorithm that consisted of the rate law, stoichiometry, and combined equations, we were able to generate data and graphs as shown in the figures above. This application was a terrific way to solve complex problems in a short amount of time.

Problem Statement 2:

The dehydrogenation of a compound (elementary kinetics) is taking place in a selective membrane reactor under isothermal conditions.



The reaction is reversible, and K_c is the equilibrium constant. The manner in which K_c (the mass transfer coefficient at volumetric flow rate v_0) increases with flow rate depends upon the flow geometry and the mass transfer dependence on velocity is given by

$$K_c = k_{c0} (v/v_0)^{1/2}$$

And the membrane transport of C is given by $k_{c0}C_c$ when permeate concentration of C is low.

1. Compare the calculated output value of FB, the molar flow rate of B for no pressure drop.

Assumptions

To successfully analyze the packed bed reactor, we must assume the following:

- Elementary Gas Phase Reaction
- The process is isothermal ($T=T_0$)
- There is a reaction occurring at the surface of the catalysts regardless of membrane transport

Identify:

Given Information:

F_{A0} (Initial Molar Concentration) = 10 kg-mol/min

v_0 (Initial Volumetric Flow rate) = 50 dm³ /min

k (rate constant) = 0.5 dm³ /kg.min

α (Constant depending on the packing bed) = 0.002 atm/kg

P_0 (Inlet pressure) = 10 atm

W (Weight Catalyst) = 200 kg

Formulate

Mole Balance

$$\frac{dX_A}{dW} = \frac{r'_A}{F_{A0}}$$

The mole balance for the packed bed reactor includes the differential value, X_A , which represents the conversion factor of species A entering the reactor. The variable W represents the Weight of the catalyst, F_{A0} is the Initial Molar flow rate of species A, and r'_A is the rate law and is dependent on the concentration of a species.

Rate Law

$$r'_A = k C_{A0}$$

The rate Law equation developed from the reaction given in the problem statement will assist in calculating the weight of the catalyst.

Stoichiometric Table:

Table 2: Problem 2 Stoichiometric Table

Symbol	Initial	Change	Remaining	Concentration
A	C_{A0}	$-C_{A0}X_A$	$C_{A0} - C_{A0}X_A$	$C_A = C_{A0} \frac{1 - X_A}{1 + \varepsilon X_A} * \frac{P}{P_0}$
B	$C_{B0} = 0$	$C_{A0}X_A$	$0 + C_{A0}X_A$	$C_B = C_{A0} \frac{X_A}{1 + \varepsilon X_A} * \frac{P}{P_0}$
C	$C_{C0} = 0$	$C_{A0}X_A$	$0 + 1/2 C_{A0}X_A$	$C_C = C_{A0} \frac{X_A}{2(1 + \varepsilon X_A)} * \frac{P}{P_0}$

Polymath Results

```
# Kinetics Homework 2
# Kennedy Dent
# Dr. Shamim
# Problem 2

FA0 = 10 # Initial Molar Flow rate (kgmol/min)
v0 = 50 # Volumetric Flow rate (dm³/min)
CA0 = FA0 / v0 # Initial Concentration of species A (kgmol/dm³)
rA = k * CA0 * (1 - XA) / (1 + eps * XA) * y # Rate Law equation
y = (1 - alpha * W) ^ 0.5 # P/P0
d(XA)/d(W) = rA / FA0 # Mole Balance for Packed Bed
W(0) = 0
Wf = 200 # Weight of the catalyst (kg)
XA(0) = 0
eps = yA0 * delta
delta = 0.5
yA0 = 1 # Mole fraction of A in the Gas phase
alpha = 0.002 # (atm/kg)
k = 0.5 # rate constant 9 dm³/kg min
d(p)/d(W) = -alpha * (1 + eps * XA / 2 * (1 - alpha * W) ^ 0.5) # Differential form of Ergun's Equation
p(0) = 1
P0 = 10 # pressure (atm)
P = P0 * (1 - alpha * W) ^ 0.5 # Final Pressure (atm)
FB = FA0 * XA # Molar Flow Rate of B
```

Figure 4: Generated values for the packed bed reactor using the Polymath Algorithm

The Polymath application allowed me to input the algorithms, equations, and initial values to solve key parameters for the packed bed reactor like problem 1. However, the focus of this problem was to calculate F_B and compare its values with and without pressure drop. All variables were clearly defined in the application and the Ergun's equation was used to relate pressure drop and the catalyst weight, and find the molar flow rate of species B.

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	W	0	0	200.	200.
2	XA	0	0	0.7640435	0.7640435
3	p	1.	0.5562922	1.	0.5562922
4	FA0	10.	10.	10.	10.
5	v0	50.	50.	50.	50.
6	CA0	0.2	0.2	0.2	0.2
7	k	0.5	0.5	0.5	0.5
8	alpha	0.002	0.002	0.002	0.002
9	yA0	1.	1.	1.	1.
10	delta	0.5	0.5	0.5	0.5
11	eps	0.5	0.5	0.5	0.5
12	y	1.	0.7745967	1.	0.7745967
13	rA	0.1	0.0132249	0.1	0.0132249
14	P0	10.	10.	10.	10.
15	P	10.	7.745967	10.	7.745967
16	FB	0	0	7.640435	7.640435

Figure 5: Generated values for the packed bed reactor using the Polymath Algorithm

Pressure Drop

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	W	0	0	200.	200.
2	XA	0	0	0.7979666	0.7979666
3	FA0	10.	10.	10.	10.
4	vo	50.	50.	50.	50.
5	CA0	0.2	0.2	0.2	0.2
6	k	0.5	0.5	0.5	0.5
7	delta	0.5	0.5	0.5	0.5
8	YAO	1.	1.	1.	1.
9	eps	0.5	0.5	0.5	0.5
10	FB	0	0	7.979666	7.979666
11	alpha	0.002	0.002	0.002	0.002
12	Po	10.	10.	10.	10.
13	rA	0.1	0.0144414	0.1	0.0144414
14	P	10.	7.745967	10.	7.745967

Figure 6: Generated values for the packed bed reactor using the Polymath Algorithm

Without Pressure Drop

Conclusion

The results generated by Polymath allowed us to correlate the effect of pressure drop on our molar flow rates. From the data we can see that FB decreased when pressure drop is present. We were able to input differential equations, rate law equations, and even Ergun's Equation to allow Polymath to create an algorithm and solve both problems 1 and 2. Figures 5 and 6 show the molar flow rate going from 7.98 kg-mol/min without pressure drop to 7.64 kg-mol/min with pressure drop. The driving force for this change in flow rate is pressure.

AVERAGE

Average Student Original Graded Assignment

For the elementary gas-phase reaction: $2A + B \rightarrow 2C$, $k_1 = 0.0001 \text{ min}^{-1}$

is carried out isothermally at 400 K in a flow reactor with the pressure drop due to friction neglected (i.e., $\Delta P = 0$) (from gas-phase) and the reaction energy is negligible. Feed at 1 atm and 400 K. The feed is 20% A, 10% B, and 70% inert.

At 10 atm and 400 K, the feed rate is 0.5 mol/min of A, B, and inert.

Use the algorithm for steady flow rate to determine the problem. (Fig. 8-1, 8-2, 8-3, 8-4, 8-5, 8-6, 8-7, 8-8, 8-9, 8-10, 8-11, 8-12, 8-13, 8-14, 8-15, 8-16, 8-17, 8-18, 8-19, 8-20, 8-21, 8-22, 8-23, 8-24, 8-25, 8-26, 8-27, 8-28, 8-29, 8-30, 8-31, 8-32, 8-33, 8-34, 8-35, 8-36, 8-37, 8-38, 8-39, 8-40, 8-41, 8-42, 8-43, 8-44, 8-45, 8-46, 8-47, 8-48, 8-49, 8-50, 8-51, 8-52, 8-53, 8-54, 8-55, 8-56, 8-57, 8-58, 8-59, 8-60, 8-61, 8-62, 8-63, 8-64, 8-65, 8-66, 8-67, 8-68, 8-69, 8-70, 8-71, 8-72, 8-73, 8-74, 8-75, 8-76, 8-77, 8-78, 8-79, 8-80, 8-81, 8-82, 8-83, 8-84, 8-85, 8-86, 8-87, 8-88, 8-89, 8-90, 8-91, 8-92, 8-93, 8-94, 8-95, 8-96, 8-97, 8-98, 8-99, 9-00)

Calculate the space-time and conversion for a CSTR reactor.

1. Feed

Feed rate: $F_{A0} = 0.5 \text{ mol/min}$

Feed composition: $y_{A0} = 0.2, y_{B0} = 0.1, y_{I0} = 0.7$

Feed pressure: $P_0 = 1 \text{ atm}$

Feed temperature: $T_0 = 400 \text{ K}$

Feed volume: $V_0 = \frac{F_{A0}}{P_0} = 0.5 \text{ m}^3/\text{min}$

Feed density: $\rho_0 = \frac{F_{A0}}{V_0} = 1 \text{ mol/m}^3$

Feed concentration: $C_{A0} = \frac{F_{A0}}{V_0} = 1 \text{ mol/m}^3$

Feed rate of A: $F_{A0} = 0.5 \text{ mol/min}$

Feed rate of B: $F_{B0} = 0.1 \text{ mol/min}$

Feed rate of inert: $F_{I0} = 0.7 \text{ mol/min}$

Feed rate of total: $F_{T0} = 1.3 \text{ mol/min}$

Feed rate of A: $F_{A0} = 0.5 \text{ mol/min}$

Feed rate of B: $F_{B0} = 0.1 \text{ mol/min}$

Feed rate of inert: $F_{I0} = 0.7 \text{ mol/min}$

Feed rate of total: $F_{T0} = 1.3 \text{ mol/min}$

Feed rate of A: $F_{A0} = 0.5 \text{ mol/min}$

Feed rate of B: $F_{B0} = 0.1 \text{ mol/min}$

Feed rate of inert: $F_{I0} = 0.7 \text{ mol/min}$

Feed rate of total: $F_{T0} = 1.3 \text{ mol/min}$

2. Reaction

Reaction: $2A + B \rightarrow 2C$

Rate law: $r_A = -k_1 C_A^2 C_B$

Rate constant: $k_1 = 0.0001 \text{ min}^{-1}$

Reaction order: 3

Reaction rate: $r_A = -k_1 C_A^2 C_B$

Reaction rate: $r_B = -\frac{1}{2} k_1 C_A^2 C_B$

Reaction rate: $r_C = k_1 C_A^2 C_B$

Reaction rate: $r_I = 0$

Reaction rate: $r_A = -k_1 C_A^2 C_B$

Reaction rate: $r_B = -\frac{1}{2} k_1 C_A^2 C_B$

Reaction rate: $r_C = k_1 C_A^2 C_B$

Reaction rate: $r_I = 0$

3. CSTR

Space-time: $\tau = \frac{V}{V_0}$

Conversion: $X = \frac{F_{A0} - F_A}{F_{A0}}$

Conversion: $X = \frac{F_{B0} - F_B}{F_{B0}}$

Conversion: $X = \frac{F_{I0} - F_I}{F_{I0}}$

Conversion: $X = \frac{F_{T0} - F_T}{F_{T0}}$

Conversion: $X = \frac{F_{A0} - F_A}{F_{A0}}$

Conversion: $X = \frac{F_{B0} - F_B}{F_{B0}}$

Conversion: $X = \frac{F_{I0} - F_I}{F_{I0}}$

Conversion: $X = \frac{F_{T0} - F_T}{F_{T0}}$

Conversion: $X = \frac{F_{A0} - F_A}{F_{A0}}$

Conversion: $X = \frac{F_{B0} - F_B}{F_{B0}}$

Conversion: $X = \frac{F_{I0} - F_I}{F_{I0}}$

Conversion: $X = \frac{F_{T0} - F_T}{F_{T0}}$

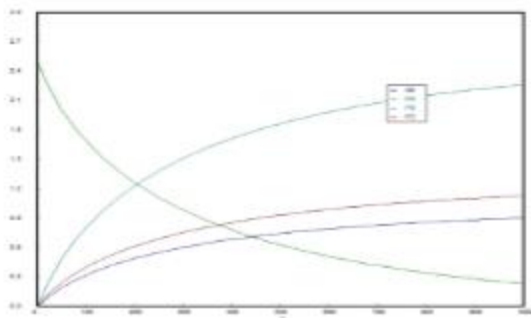


Figure 1. F_A, F_B, F_C, X vs. space

```
# Jacques Center
# Dr. Nabila Shamm
# Homework Problem 6-4B

dXA/dV = -rA / FA0
rA = -k * CA
CA = CA0 * (1 - XA) / (1 + e * XA)
k = 0.004
e = 2
FA0 = 2.5
CA0 = 0.3
XA(0) = 0
V(0) = 0
Vf = 1000
Tau = V / v0
v0 = 5.33

# FLOW RATES
dFA/dV = rA
FA(0) = 2.5
dFB/dV = -rA
FB(0) = 0
dFC/dV = rA / 2
FC(0) = 0
```

Figure 1. Polymath Coding

The polymath graphs look good.

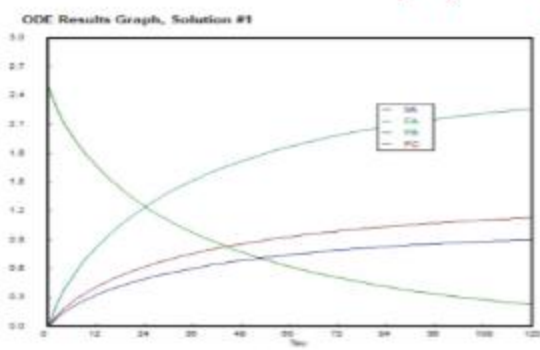


Figure 3. F_A, F_B, F_C, X vs. space time

Step	Time	FA	FB	FC	X	TA	VB	VC	VD	VE	VF	VG	VH	VI	VJ	VK	VL	VM	VN	VO	VP	VQ	VR	VS	VT	VU	VV	VW	VX	VY	VZ	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE	BF	BG	BH	BI	BJ	BK	BL	BM	BN	BO	BP	BQ	BR	BS	BT	BU	BV	BW	BX	BY	BZ	CA	CB	CC	CD	CE	CF	CG	CH	CI	CJ	CK	CL	CM	CN	CO	CP	CQ	CR	CS	CT	CU	CV	CW	CX	CY	CZ	DA	DB	DC	DD	DE	DF	DG	DH	DI	DJ	DK	DL	DM	DN	DO	DP	DQ	DR	DS	DT	DU	DV	DW	DX	DY	DZ	EA	EB	EC	ED	EE	EF	EG	EH	EI	EJ	EK	EL	EM	EN	EO	EP	EQ	ER	ES	ET	EU	EV	EW	EX	EY	EZ	FA	FB	FC	FD	FE	FF	FG	FH	FI	FJ	FK	FL	FM	FN	FO	FP	FQ	FR	FS	FT	FU	FV	FW	FX	FY	FZ	GA	GB	GC	GD	GE	GF	GG	GH	GI	GJ	GK	GL	GM	GN	GO	GP	GQ	GR	GS	GT	GU	GV	GW	GX	GY	GZ	HA	HB	HC	HD	HE	HF	HG	HH	HI	HJ	HK	HL	HM	HN	HO	HP	HQ	HR	HS	HT	HU	HV	HW	HX	HY	HZ	IA	IB	IC	ID	IE	IF	IG	IH	II	IJ	IK	IL	IM	IN	IO	IP	IQ	IR	IS	IT	IU	IV	IW	IX	IY	IZ	JA	JB	JC	JD	JE	JF	JG	JH	JI	JJ	JK	JL	JM	JN	JO	JP	JQ	JR	JS	JT	JU	JV	JW	JX	JY	JZ	KA	KB	KC	KD	KE	KF	KG	KH	KI	KJ	KL	KM	KN	KO	KP	KQ	KR	KS	KT	KU	KV	KW	KX	KY	KZ	LA	LB	LC	LD	LE	LF	LG	LH	LI	LJ	LK	LM	LN	LO	LP	LQ	LR	LS	LT	LU	LV	LW	LX	LY	LZ	MA	MB	MC	MD	ME	MF	MG	MH	MI	MJ	MK	ML	MM	MN	MO	MP	MQ	MR	MS	MT	MU	MV	MW	MX	MY	MZ	NA	NB	NC	ND	NE	NF	NG	NH	NI	NJ	NK	NL	NO	NP	NQ	NR	NS	NT	NU	NV	NW	NX	NY	NZ	OA	OB	OC	OD	OE	OF	OG	OH	OI	OJ	OK	OL	OM	ON	OO	OP	OQ	OR	OS	OT	OU	OV	OW	OX	OY	OZ	PA	PB	PC	PD	PE	PF	PG	PH	PI	PJ	PK	PL	PM	PN	PO	PP	PQ	PR	PS	PT	PU	PV	PW	PX	PY	PZ	QA	QB	QC	QD	QE	QF	QG	QH	QI	QJ	QK	QL	QM	QN	QO	QP	QQ	QR	QS	QT	QU	QV	QW	QX	QY	QZ	RA	RB	RC	RD	RE	RF	RG	RH	RI	RJ	RK	RL	RM	RN	RO	RP	RQ	RR	RS	RT	RU	RV	RW	RX	RY	RZ	SA	SB	SC	SD	SE	SF	SG	SH	SI	SJ	SK	SL	SM	SN	SO	SP	SQ	SR	SS	ST	SU	SV	SW	SX	SY	SZ	TA	TB	TC	TD	TE	TF	TG	TH	TI	TJ	TK	TL	TM	TN	TO	TP	TQ	TR	TS	TT	TU	TV	TW	TX	TY	TZ	UA	UB	UC	UD	UE	UF	UG	UH	UI	UJ	UK	UL	UM	UN	UO	UP	UQ	UR	US	UT	UU	UV	UW	UX	UY	UZ	VA	VB	VC	VD	VE	VF	VG	VH	VI	VJ	VK	VL	VM	VN	VO	VP	VQ	VR	VS	VT	VU	VV	VW	VX	VY	VZ	WA	WB	WC	WD	WE	WF	WG	WH	WI	WJ	WK	WL	WM	WN	WO	WP	WQ	WR	WS	WT	WU	WV	WW	WX	WY	WZ	XA	XB	XC	XD	XE	XF	YG	YH	YI	YJ	YK	YL	YM	YN	YO	YP	YQ	YR	YS	YT	YU	YV	YW	YX	YY	YZ	ZA	ZB	ZC	ZD	ZE	ZF	ZG	ZH	ZI	ZJ	ZK	ZL	ZM	ZN	ZO	ZP	ZQ	ZR	ZS	ZT	ZU	ZV	ZW	ZX	ZY	ZZ	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE	BF	BG	BH	BI	BJ	BK	BL	BM	BN	BO	BP	BQ	BR	BS	BT	BU	BV	BW	BX	BY	BZ	CA	CB	CC	CD	CE	CF	CG	CH	CI	CJ	CK	CL	CM	CN	CO	CP	CQ	CR	CS	CT	CU	CV	CW	CX	CY	CZ	DA	DB	DC	DD	DE	DF	DG	DH	DI	DJ	DK	DL	DM	DN	DO	DP	DQ	DR	DS	DT	DU	DV	DW	DX	DY	DZ	EA	EB	EC	ED	EE	EF	EG	EH	EI	EJ	EK	EL	EM	EN	EO	EP	EQ	ER	ES	ET	EU	EV	EW	EX	EY	EZ	FA	FB	FC	FD	FE	FF	FG	FH	FI	FJ	FK	FL	FM	FN	FO	FP	FQ	FR	FS	FT	FU	FV	FW	FX	FY	FZ	GA	GB	GC	GD	GE	GF	GG	GH	GI	GJ	GK	GL	GM	GN	GO	GP	GQ	GR	GS	GT	GU	GV	GW	GX	GY	GZ	HA	HB	HC	HD	HE	HF	HG	HH	HI	HJ	HK	HL	HM	HN	HO	HP	HQ	HR	HS	HT	HU	HV	HW	HX	HY	HZ	IA	IB	IC	ID	IE	IF	IG	IH	II	IJ	IK	IL	IM	IN	IO	IP	IQ	IR	IS	IT	IU	IV	IW	IX	IY	IZ	JA	JB	JC	JD	JE	JF	JG	JH	JI	JJ	JK	JL	JM	JN	JO	JP	JQ	JR	JS	JT	JU	JV	JW	JX	JY	JZ	KA	KB	KC	KD	KE	KF	KG	KH	KI	KJ	KL	KM	KN	KO	KP	KQ	KR	KS	KT	KU	KV	KW	KX	KY	KZ	LA	LB	LC	LD	LE	LF	LG	LH	LI	LJ	LK	LM	LN	LO	LP	LQ	LR	LS	LT	LU	LV	LW	LX	LY	LZ	MA	MB	MC	MD	ME	MF	MG	MH	MI	MJ	MK	ML	MM	MN	MO	MP	MQ	MR	MS	MT	MU	MV	MW	MX	MY	MZ	NA	NB	NC	ND	NE	NF	NG	NH	NI	NJ	NK	NL	NO	NP	NQ	NR	NS	NT	NU	NV	NW	NX	NY	NZ	OA	OB	OC	OD	OE	OF	OG	OH	OI	OJ	OK	OL	OM	ON	OO	OP	OQ	OR	OS	OT	OU	OV	OW	OX	OY	OZ	PA	PB	PC	PD	PE	PF	PG	PH	PI	PJ	PK	PL	PM	PN	PO	PP	PQ	PR	PS	PT	PU	PV	PW	PX	PY	PZ	QA	QB	QC	QD	QE	QF	QG	QH	QI	QJ	QK	QL	QM	QN	QO	QP	QQ	QR	QS	QT	QU	QV	QW	QX	QY	QZ	RA	RB	RC	RD	RE	RF	RG	RH	RI	RJ	RK	RL	RM	RN	RO	RP	RQ	RR	RS	RT	RU	RV	RW	RX	RY	RZ	SA	SB	SC	SD	SE	SF	SG	SH	SI	SJ	SK	SL	SM	SN	SO	SP	SQ	SR	SS	ST	SU	SV	SW	SX	SY	SZ	TA	TB	TC	TD	TE	TF	TG	TH	TI	TJ	TK	TL	TM	TN	TO	TP	TQ	TR	TS	TT	TU	TV	TW	TX	TY	TZ	UA	UB	UC	UD	UE	UF	UG	UH	UI	UJ	UK	UL	UM	UN	UO	UP	UQ	UR	US	UT	UU	UV	UW	UX	UY	UZ	VA	VB	VC	VD	VE	VF	VG	VH	VI	VJ	VK	VL	VM	VN	VO	VP	VQ	VR	VS	VT	VU	VV	VW	VX	VY	VZ	WA	WB	WC	WD	WE	WF	WG	WH	WI	WJ	WK	WL	WM	WN	WO	WP	WQ	WR	WS	WT	WU	WV	WW	WX	WY	WZ	XA	XB	XC	XD	XE	XF	YG	YH	YI	YJ	YK	YL	YM	YN	YO	YP	YQ	YR	YS	YT	YU	YV	YW	YX	YY	YZ	ZA	ZB	ZC	ZD	ZE	ZF	ZG	ZH	ZI	ZJ	ZK	ZL	ZM	ZN	ZO	ZP	ZQ	ZR	ZS	ZT	ZU	ZV	ZW	ZX	ZY	ZZ
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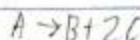
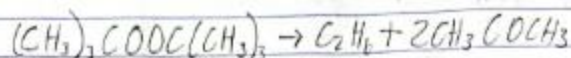
85

BELOW AVERAGE

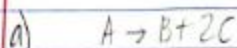
Below Average Student Original Graded Assignment

HW #3

P6-4B



Elementary Gas Reaction



$$V = \frac{F_{A0} \cdot (-r_A - k C_A)}{-r_A}$$

$$C_A = \frac{C_{A0}(1-x)}{(1+Ex)}, \quad E = Y_A, \quad S = (1)(2+1-1) = 2$$

$$C_{A0} = \frac{P_{A0}}{RT} = \frac{10}{(0.082)(400)} = 0.3 \text{ mol/dm}^3$$

$$V = F_{A0} \int_0^x \frac{dx}{-r_A} = \frac{F_{A0}}{k C_{A0}} \int_0^x \frac{1+Ex}{1-x} dx$$

$$= \frac{F_{A0}}{k C_{A0}} \left[(1+E) \ln \frac{1}{1-x} - Ex \right]$$

$$= \left(\frac{(2.5 \text{ mol/min})}{(0.044 \text{ min}^{-1})(0.3 \text{ mol/dm}^3)} \right) \left(\frac{1 + \ln -1.8}{1 - 0.9} \right)$$

$$= (139.4 \text{ dm}^3) (5.11)$$

$$V = 967 \text{ dm}^3$$

$$V = \frac{F_{A0} \cdot (1+Ex)}{C_{A0} \cdot k \cdot (1-x)} \quad \therefore k = 10^{-4} e^{\frac{8500}{8.31} \left(\frac{1}{32.3} - \frac{1}{400} \right)} = 0.044$$

$$V = \frac{(2.5 \text{ mol/min}) (0.9) (1 + 0.9(0.9))}{(0.044 \text{ min}^{-1}) (0.3 \text{ mol/dm}^3) (1 - 0.9)} = \boxed{4772 \text{ dm}^3}$$

b) Space time

$$F_{A0} = C_{A0} V_0$$

$$V_0 = \frac{F_{A0}}{C_{A0}}$$

$$V_0 = \frac{2.5 \text{ mol/min}}{0.3 \text{ mol/dm}^3}$$

$$\tau = \frac{V}{V_0}$$

$$\tau = \frac{4772 \text{ dm}^3}{8.3 \text{ dm}^3/\text{min}}$$

$$\tau = 574.93 \text{ min}$$

$$V_0 = 8.3 \text{ dm}^3/\text{min}$$

P6-7a

Mole

$$\frac{dF_B}{dw} = r_B$$

$$\frac{dF_C}{dw} = r_C$$

$$\frac{dF_D}{dw} = -R_D + r_D$$

Balance:

$$\frac{dF_B}{dw} = r_B$$

$$\frac{dF_C}{dw} = -r_A$$

$$\frac{dF_D}{dw} = -R_D - r_A$$

$$\text{Rate law: } -r_A = k \left[C_A C_B - \frac{C_C C_D}{K_c} \right]$$

hydrogen diffuses out the membrane $R_D = k_{H_2} [C_0 - C_{cs}]$

$$R_D = k_{H_2} C_0$$

$$\therefore -r_A = k \left(\frac{C_A C_B}{F_r} \right) \left(F_A F_B - \frac{F_C F_D}{K_c} \right)$$

$$F_A = \frac{F_{A0} (1-x)}{(1-Ex)}$$

$$F_B = \frac{F_{B0} (1-x)}{(1-Ex)}$$

$$F_C = \frac{F_{C0} + F_{A0} x}{(1-Ex)}$$

$$F_D = \frac{F_{D0} + F_{A0} x}{(1-Ex)}$$

$$E = Y_{A0} \cdot S_A$$

$$S_A = \frac{2-2}{1} = 0 \quad \therefore E = 0.5 \times 0$$

$$E = 0$$

$$F_{A0} = C_{A0} \cdot V_0 \quad C_{A0} \text{ is } 0.2 \text{ mol/dm}^3$$

$$F_{A0} = 0.2 \left(\frac{\text{mol}}{\text{dm}^3} \right) \cdot 10 \left(\frac{\text{dm}^3}{\text{min}} \right) = 2 \text{ mol/min}$$

$$F_A = 2(1-x) \text{ mol/min}$$

$$F_C = 2x \text{ (mol/min)}$$

$$F_B = 2(1-x) \text{ mol/min}$$

$$F_D = 2x \text{ (mol/min)}$$

$$a) \quad F_a = 0.85 \\ F_b = 2(1-0.85) = 0.3 \text{ (mol/min)}$$

$$F_B = 2(1-0.85) = 0.3 \text{ (mol/min)}$$

$$F_c = 2(0.85) = 1.7 \text{ mol/min}$$

$$F_p = 2(0.85) = 1.7 \text{ mol/min}$$

$$F_r = 0.3 \text{ (mol/min)} + 0.3 \text{ (mol/min)} + 1.7 \text{ (mol/min)} = 1.7 \text{ (mol/min)}$$

$$= 4 \text{ mol/min}$$

$$-r_a = k \left(\frac{C_{A0}}{F_r} \right)^2 \left(F_a F_b - \frac{F_c F_p}{K_c} \right)$$

$$= 1.37 \left(\frac{\text{dm}^3}{\text{mol} \cdot \text{kg} \cdot \text{cat} \cdot \text{min}} \right) \cdot \left[\frac{0.4 \text{ mol/dm}^3}{4 \text{ mol/min}} \right]^2 \left[1.3 \frac{\text{mol}}{\text{min}} \cdot 0.3 \frac{\text{mol}}{\text{min}} - \frac{1.7 \frac{\text{mol}}{\text{min}} \cdot 1.7}{1.47} \right]$$

$$-r_a = -0.0212 \left(\frac{\text{mol}}{\text{kg} \cdot \text{cat} \cdot \text{min}} \right)$$

$$\frac{dF_a}{dw} = r_a \quad \frac{0.3 \text{ mol/min} - 2 \frac{\text{mol}}{\text{min}}}{1 \text{ kg/cat}} = -0.0212 \left(\frac{\text{mol}}{\text{kg} \cdot \text{cat} \cdot \text{min}} \right)$$

$$w = (4.55 \text{ kg} \cdot \text{cat})$$

$$b) \quad \theta_a = -\frac{C_{A0}}{r_a} = 1$$

$$\theta_a = \frac{C_{A0}}{r_a} = \frac{0.2 \text{ mol/dm}^3}{0.2 \text{ mol/min}} = 1$$

$$\theta_c = \frac{C_{A0}}{r_c} = 0$$

$$\theta_p = \frac{C_{A0}}{r_p} = 0$$

(Since; $C_{A0} = 0$ and $r_p = 0$)

$$C_B = C_{A0} \left(\theta_a - \frac{1}{4}x \right) = 0.2 \text{ mol/dm}^3 \left(1 - \frac{1}{4}x \right) = 0.2(1-x)$$

$$C_c = C_{A0} \left(\theta_c + \frac{5}{4}x \right) = 0.2 \text{ mol/dm}^3 \left(0 + \frac{1}{4}x \right) = 0.2x$$

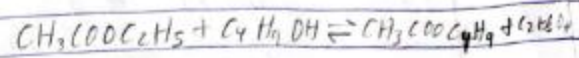
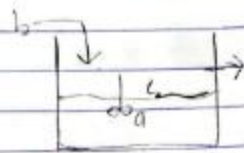
$$C_p = C_{A0} \left(\theta_p + \frac{1}{4}x \right) = 0.2 \text{ mol/dm}^3 \left(0 + \frac{1}{4}x \right) = 0.2x$$

$$K_e = \frac{C_c C_b}{C_a C_b} = \frac{(0.2x)(0.2x)}{(0.2(1-x))} = 1.44 = \frac{x^2}{(1-x)^2}$$

When x is 0.545 the conversion is 54.5%

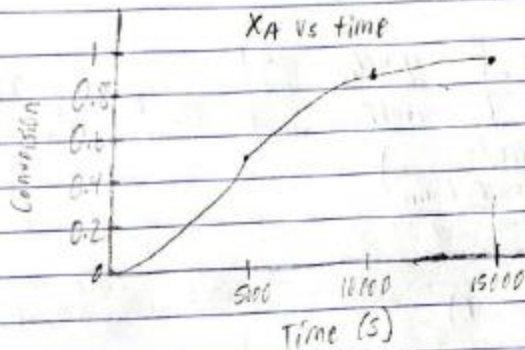
c)

P6-11B



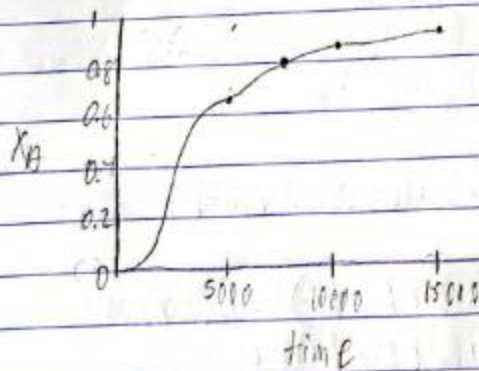
$$\frac{dC_A}{dt} = 0$$

d) $k_B (C_A - C_A^*)^2 = k_F C_A \left[\frac{F_B t}{V} - (C_A - C_A^*) \right]$



$$k_B C_A C_D = k_F C_A C_0$$

$$k_B (C_A - C_A^*)^2 = k_F C_A \left[\frac{F_B}{V} - (C_A - C_A^*) \right]$$



show the polymath results -20

Chemical Reaction Kinetics and Reactor Design CHEG 3306 PO 1 (Spring 2022)

Project 1

TOPICS COVERED IN Project 1

1. Define/Understand the Kinetics and reactor design Problem
 - a. Develop mole balance equation
 - b. Rate law and stoichiometry and combine
2. Perform detailed design of complex chemical engineering design

**Chemical Reaction Kinetics and Reactor Design CHEG 3306 PO 1
(Spring 2022)**

**Final Project # QUESTIONS, SOLUTION,
AND GRADING SCHEME**

Final Project CHEG 3306
Spring 2021 Due Date April 30, 2022

Project objectives:

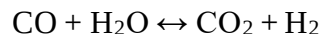
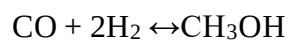
- To demonstrate your understanding of designing a packed bed reactor.
- Show that you can calculate the required design taking heat, pressure drop and changing physical properties into account.
- Design and create a plan of action that you will follow to achieve your goal.
- To reflect afterwards on your group's progress and judge how you followed your plan.

You are required to design a shell and tube packed-bed reactor for methanol synthesis. The complete problem statement follows.

1. Projects are to be tackled in groups, with one report per group. Each student will submit at the end of the project a confidential assessment of the relative contributions of the members of the group.
2. The methodology used in the design of the reactor must be clearly explained; all assumptions must be identified and evaluated; the results must be clearly presented and discussed. In particular you must have a section at the start of your report where you: "clearly explain the strategy you will follow to achieve the project's objective". Use bullet points showing the sequence of steps you planned.
3. Reports must be written in an acceptable and professional style and should not exceed 15 typed pages (including any appendices). Any polymath code you choose to include in part of your page limit. You must submit your report using Canvas.
4. All published information consulted must be appropriately referenced.
5. At the end you must have a section called "Reflection". Answer these 3 questions in the section:
 - How accurately did our group stick to the plan (there is no penalty from deviating from your plan, but describe why you deviated).
 - How would we go about the project differently if we could redo it?
 - What did we learn from doing this project (bullet points are OK).

Problem statement

A new catalyst has been proposed for the synthesis of methanol from carbon monoxide and hydrogen gas. This catalyst is reasonably active between temperatures of 330 K to about 430 K. The reactions to be considered are:



The reactions are elementary and occur in a reactor containing tubes packed with a precious metal catalyst on a silica support. Heat is removed from the reactor by generating steam on the shell side of the tubes. The feed consists of 7/15 hydrogen gas, 1/5 carbon monoxide, 1/5 carbon dioxide, and 2/15 steam. The total flow rate is 300 mol.s^{-1} . The entering pressure may be varied between 1 atm and 160 atm and the entering temperature between 300 K and 400 K. A total tubular reactor volume of 2 m^3 is to be used.

The following tasks should be completed:

1. Discuss the commercial application of this reaction in terms of the overall process, economics, process conditions, reactor types and configurations typically used, type of catalyst, typical conversion and end product usage.
2. Assuming isothermal and isobaric conditions, determine the entering conditions of temperature and pressure that will optimize the production of methanol. Hint: Do this by conducting several simulations at discrete combinations of T_0 and P_0 . First try $T_0 = 330$ at $P_0 = 40 \text{ atm}$, then try $T_0 = 380$ and $P_0 = 1 \text{ atm}$
3. Carry out a detailed reactor design of a shell and tube reactor for the optimal feed conditions determined in part 2. Pressure drop and non-isothermal effects are to be taken into account.

The shell side temperature can be controlled by adjusting the steam pressure and may be assumed constant at a value specified by you. Physical property estimation sources, techniques and assumptions should be clearly presented. The design should include the following:

- the reactor dimensions and number of tubes
 - the reactor conditions; including composition, pressure and temperature profiles (as a function of reactor length).
 - A mechanical sketch of the reactor should be included.
 - **Not required:** mechanical design of the reactor, including specification of the reactor material of construction, shell and tube wall thickness and capital cost for the design.
4. Determine the effect of variations in:
 - ratio of feed H_2 to CO ,
 - ratio of feed H_2O to CO ,
 - assumed heat transfer coefficient, U
 5. All results must be presented in SI units throughout the report.

The following results should be tabulated in your report:

Inlet temperature [K]
 Outlet temperature [K]
 Inlet pressure [Pa]
 Outlet pressure [Pa]
 Maximum tube-side temperature [K]
 Location from inlet of maximum temperature [m]
 Methanol production rate [kg.s⁻¹]
 Reactor length [m]
 Total inlet concentration, CT0 at 330K
 Rate constant, k1 at 330K
 Equilibrium constant KC,1 at 330K
 Rate constant, k2 at 330K
 Equilibrium constant KC,2 at 330K
 Heat of reaction for reaction 1 at 330K
 Heat of reaction for reaction 2 at 330K

The following results for Reactor in and Reactor out in a tabular form must be presented

Flow [mol.s⁻¹]
 Pressure [Pa]
 Temperature [K]
 CO (mole fraction)
 H2
 CO2
 CH3OH
 H2O

If you are using MATLAB, A working set of MATLAB files must be emailed to the instructor with submission of your final report. These MATLAB files must generate the final profiles used to obtain the flows, pressure, temperature and mol fractions in the above tables. Non-working code, or code that does not lead to the values in the table will lead to a penalty in the grade.

Additional problem information Thermodynamic and rate data T is in Kelvin, but R = 1.987 cal.mol⁻¹ .K⁻¹ . The subscript 1 refers to the methanol reaction, while subscript 2 refers to the water-gas shift reaction. V = 40 dm³

$$K_1 = 131667(0.001987T)^2 \exp \left[\frac{30620}{R} \left(\frac{1}{T} - \frac{1}{298} \right) \right] \left[\frac{dm^3}{mol} \right]^2$$

$$K_2 = 103943 \exp \left[\frac{9834}{R} \left(\frac{1}{T} - \frac{1}{298} \right) \right]$$

$$k_1 = 0.933 \times 10^{-6} \exp \left[2.5 \left(\frac{31400}{R} \left(\frac{1}{330} - \frac{1}{T} \right) \right) \right] \left[\left(\frac{dm^3}{mol} \right)^2 S^{-1} \right]$$

$$k_2 = 0.636 \times 10^{-6} \exp \left[\frac{18000}{R} \left(\frac{1}{300} - \frac{1}{T} \right) \right] \left[\frac{dm^3}{mol.s} \right]$$

ABOVE AVERAGE

Above Average Student Original Graded Assignment

Prairie View A&M University
Roy G. Perry College of Engineering
Department: Chemical Engineering



CHEG 3306- P01
Chemical Reaction Kinetics and Reactor Design
Final Project

Submitted by:
Jazmaine Carter
Dynasty Stephenson
Edgar Mendoza

Due Date: 05-6-22

Submitted to: Dr. Shamim

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Project Objectives

- To demonstrate your understanding of designing a packed bed reactor.
- Show that you can calculate the required design by taking heat, pressure drop, and changing physical properties into account.
- Design and create a plan of action that you will follow to achieve your goal.
- To reflect afterward on your group's progress and judge how you followed your plan.

Project Tasks

1. Discuss the commercial application of this reaction in terms of the overall process, economics, process conditions, reactor types and configurations typically used, type of catalyst, typical conversion, and end product usage.
2. Assuming isothermal and isobaric conditions, determine the entering conditions of temperature and pressure that will optimize the production of methanol. *Hint: Do this by conducting several simulations at discrete combinations of T_0 and P_0 . First try $T_0 = 330$ at $P_0 = 40$ atm, then try $T_0 = 380$ and $P_0 = 1$ atm).*
3. Carry out a detailed reactor design of a shell and tube reactor for the optimal feed conditions determined in part 2. Pressure drop and non-isothermal effects are to be taken into account. The shell side temperature can be controlled by adjusting the steam pressure and may be assumed constant at a value specified by you. Physical property estimation sources, techniques, and assumptions should be clearly presented. The design should include the following:
 - the reactor dimensions and number of tubes
 - the reactor conditions; including composition, pressure, and temperature profiles (as a function of reactor length).
 - A mechanical sketch of the reactor should be included.
4. Determine the effect of variations in:
 - ratio of feed H_2 to CO , ratio of feed H_2O to CO , assumed heat transfer coefficient, U
5. All results must be presented in SI units throughout the report.

Plan of action

1. Discuss schedule conflicts with group members.
2. Discuss group project tasks and deadlines.
3. Assign group leader: **Jazmaine Carter**
4. Research potential sources for data.
5. Write down any questions for Dr. Shamim about the project.
6. Schedule 1st meeting with Dr. Shamim. (4-12-22) **zoom**.
7. Review and make corrections after meeting with Dr. Shamim.
8. Schedule 2nd meeting with Dr. Shamim (4-26-22) **in person**.
9. Consult with Dr. Shamim for calculation/Equation verifications.
10. Consult with Dr. Shamim for schematic diagram verification.
11. Gather all given and calculated data for polymath
12. Run polymath program
13. Collect all data from polymath program
14. Finish writing report
15. Start PowerPoint for presentation
16. DONE!

Executive Summary

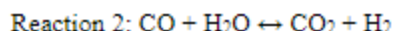
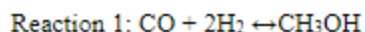
Methanol synthesis reaction is an exothermic reaction that is highly possible source for alternative energy. To produce methanol is by using a mixture of carbon monoxide, and hydrogen under high pressure and temperature. For our process, Cu/ZnO will be used for the reactor catalyst for an optimal production. The synthesis of methanol is dependent on the temperature, pressure and catalyst used. Methanol is produced through the catalytic hydrogenation of CO. The overall design is executing a Packed Bed Reactor (PBR). A lot of companies use PBRs because the reactor is a good mixer, uniformity of temperature, catalyst can be continuously regenerated and can get a higher conversion per weight of catalyst compared to other catalytic reactors. The importance of designing a PBR is mass transfer and heat transfer. It is important to optimize heat transfer through the PBR because of cost of the equipment. The catalyst should be chosen wisely because it has effect on the mass and energy transfer.

Introduction

Methanol is a toxic, colorless, volatile flammable simplest alcohol used commonly for everyday products including plastics, paints, car parts, etc. This alcohol is a clean energy resource and is produced at various companies by using different techniques to produce the best quality of methanol. One of the most current ways to produce methanol is by using three

compounds: carbon dioxide, carbon monoxide, and hydrogen. After researching different catalyst, the most effective for the reactor to make as much product is Cu/ZnO. Using a high temperature and pressure with our chosen catalyst, the reaction can produce the desired optimal product methanol.

The synthesis of methanol occurs in two different steps. The steps are as follows:



In Reaction 1, carbon monoxide reaction with hydrogen in a hydrogenation reaction producing methanol. In Reaction 2, carbon monoxide reacts with water and produces carbon dioxide and hydrogen gas. By using these steps will accomplish the synthesis of methanol. According to our research, companies use these steps as well as various alternative methods to produce methanol.

Overview

Our project that we are tasked with is executing the algorithms, research, and Polymath for methanol synthesis using a shell and tube packed bed reactor. First, we had to do in depth research to determine which catalyst would best suit the production of methanol. There was numerous catalyst that could've been chosen for this process, but we chose Cu/ZnO specifically for a desired optimal production of methanol. Throughout the report will demonstrate why we chose our catalyst, calculation steps of mole balance, rate law, stoichiometry, molar flow rate, importance of our catalyst and the process in a general aspect.

Problem Statement

A new catalyst has been proposed for the synthesis of methanol from carbon monoxide and hydrogen gas. This catalyst is reasonably active between temperatures of 330 K to about 430 K. The reactions to be considered are:



The reactions are **elementary** and occur in a reactor containing **tubes packed** with a precious **metal catalyst** on a **silica support**. Heat is removed from the reactor by generating steam on the shell side of the tubes. The **feed** consists of **7/15 hydrogen gas**, **1/5 carbon monoxide**, **1/5 carbon dioxide**, and **2/15 steam**. The **total flow rate** is **300 mol/ s**. The **entering pressure** may be **varied** between **1 atm** and **160 atm** and the **entering temperature** between **300 K** and **400 K**. A **total tubular reactor volume** of **2m³** is to be used.

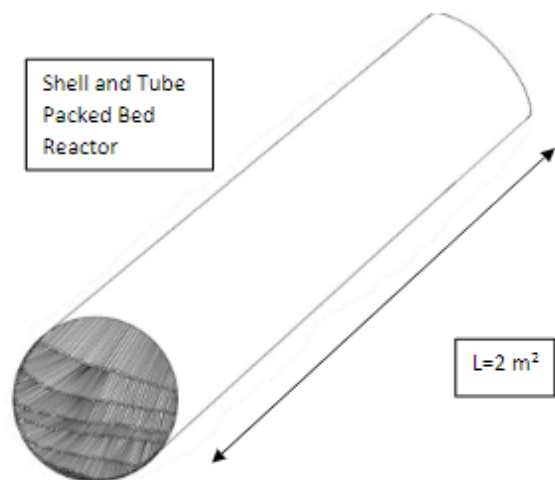


Figure 1. Schematic Diagram of Shell-Tube Packed Bed Reactor

Assumption: The tubes use up all the space in the reactor and therefore we can consider it the overall area of reactor.

Givens	
- Catalyst active between temperatures of 330K and 430K. - Feed consists of: $H_2(g) = 7/15 = .47$ $CO(g) = 1/5 = .2$ $CO_2(g) = 1/5 = .2$ $H_2O(g) = 2/15 = .13$ $FT = 300 \text{ mol/s}$ $P_o = 1 \text{ atm} - 160 \text{ atm}$ $= 101325 \text{ Pa} - 1.6E+7 \text{ Pa}$ $T_o = 300K - 400K$ - Total tubular reactor volume $(V) = 2m^3$	Additional Problem Information $R = 1.987 \text{ cal/mol}^*K$ $K_1 = 131667(.001987T)^2 \exp \left[\frac{30620}{R} \left(\frac{1}{T} - \frac{1}{298} \right) \right] \left[\frac{dm^3}{mol} \right]^2$ $K_2 = 103943 \exp \left[\frac{9834}{R} \left(\frac{1}{T} - \frac{1}{298} \right) \right]$ $k_1 = .933 \times 10^{-6} \exp \left[2.5 \left(\frac{31400}{R} \left(\frac{1}{330} - \frac{1}{T} \right) \right) \right] \left[\frac{dm^3}{s} \right]^2$ $k_2 = .636 \times 10^{-6} \exp \left[\frac{1800}{R} \left(\frac{1}{300} - \frac{1}{T} \right) \right] \left[\frac{dm^3}{mol \cdot s} \right]$ Reactor equipment data - Catalyst bed void fraction (Φ) = 40% - Catalyst density (ρ_c): 1600 kg/m^3 - Tube diameter (i.d.): $3.81 \text{ cm} = .0381m$ - Overall heat transfer coefficient (U): $631W/m^*K$ - Tube diameter (o.d.): $4.20cm = .042 m$ - Shell side water temperature: $373K$ - Catalyst particle size: $5mm = .005 m$ - Average gas viscosity (μ), assumed constant over all temperature: $7.5 \times 10^{-6} \text{ Pa} \cdot s$ - Number of tubes in the heat exchanger: 250 tubes

5

Mole Balance	Rate Law	
$\frac{dFA}{dW} = r'A$	$-r'A_1 = k_1 C_A C_B^2$ $-r'A_f = k_1 C_A C_B^2$ $r'A_f = -k_1 C_A C_B^2$ $r'A_r = k_1 C_C$ $r'A_{net} = r'A_f + r'A_r$ Hence, $r'A = -k_1 C_A C_B^2 + k_1 C_C$ But we need $-r'A$ Hence, $-r'A = k_1 C_A C_B^2 - k_1 C_C$ Note: $K_{C1} = \frac{k_1}{k_{-1}}$ Hence, $-r'A = k_1 [C_A C_B^2 - \frac{C_C}{K_{C1}}]$	$-r'D_2 = k_2 C_A C_D$ $-r'D_f = k_2 C_A C_D$ $r'D_f = -k_2 C_A C_D$ $r'D_r = k_2 C_E C_B$ $r'D_{net} = r'D_f + r'D_r$ Hence, $r'D = -k_2 C_A C_D + k_2 C_E C_B$ But we need $-r'D$ Hence, $-r'D = k_2 C_A C_D - k_2 C_E C_B$ Note: $K_{C2} = \frac{k_2}{k_{-2}}$ Hence, $-r'D = k_2 [C_A C_D - \frac{C_E C_B}{K_{C2}}]$
$\frac{dFB}{dW} = r'B$		
$\frac{dFC}{dW} = r'C$		
$\frac{dFD}{dW} = r'D$		
$\frac{dFE}{dW} = r'E$	Relative Rates: $r'B_1 = 2(r'A_1), r'C_1 = -r'A_1$	Relative Rates: $r'A_2 = r'D_2, r'E_2 = -r'D_2, r'B_2 = -r'D_2$

Table 1

Net Rates	Stoichiometry	Calculate: Molar Flow rates
$r'A = r'A_1 + r'A_2$ $r'B = r'B_1 + r'B_2$ $r'C = r'C_1$ $r'D = r'D_2$ $r'E = r'E_2$ Therefore, $r'A = -k_1 C_A C_B^2 - k_2 C_A C_D$ $r'B = (2)(-k_1 C_A C_B^2) + k_2 C_A C_D$ $r'C = k_1 C_A C_B^2$ $r'D = -k_2 C_A C_D$ $r'E = k_2 C_A C_D$	$CA = CTO \frac{FA}{FT} P$ $CB = CTO \frac{FB}{FT} P$ $CC = CTO \frac{FC}{FT} P$ $CD = CTO \frac{FD}{FT} P$ $CE = CTO \frac{FE}{FT} P$ Note: $p = \frac{P}{P_s}$; $\frac{dP}{dW} = \frac{-\beta o}{A(1-\phi)\rho c} \frac{P_o}{P} \frac{FT}{FTO}$ $FT = FA + FB + FC + FD + FE$	$FA = CO = (\frac{1}{5})(300 \text{ mol/s}) = 60 \text{ mol/s}$ $FB = H_2 = ((300 \text{ mol/s}) = 140 \text{ mol/s}$ $FC = CO_2 = (\frac{1}{5})(300 \text{ mol/s}) = 60 \text{ mol/s}$ $FD = H_2O = (\frac{7}{15})(300 \text{ mol/s}) = 40 \text{ mol/s}$ Molar Masses: $CO = 28.01 \text{ g/mol}$ $H_2 = 2.02 \text{ g/mol}$ $CO_2 = 44.01 \text{ g/mol}$ $H_2O = 18.02 \text{ g/mol}$ For mass flow rate ($\dot{m}$): We use $\dot{m} = (\text{mass}) (\text{flowrate})$ $\dot{m}_{H_2} = (.00202 \text{ kg/mol}) (140 \text{ mol/s}) = .29 \text{ kg/s}$ $\dot{m}_{CO} = (.02801 \text{ kg/mol}) (60 \text{ mol/s}) = 1.7 \text{ kg/s}$ $\dot{m}_{CO_2} = (.04401 \text{ kg/mol}) (60 \text{ mol/s}) = 2.6 \text{ kg/s}$ $\dot{m}_{H_2O} = (.01802 \text{ kg/mol}) (40 \text{ mol/s}) = .72 \text{ kg/s}$ TOTAL $\dot{m}$: 5.31 kg/s

Table 2

Calculations for Area, β_0 , and α	
For Area of Pipe/heat exchanger: $A = n \frac{\pi D_i^2}{4}$ Since, $D_i = .0381\text{m}$ $n = 250$ tubes Hence, $A = .285\text{m}^2$ For overall area of heat exchanger: <i>Note: we assumed the tubes occupy all the space inside the reactor and therefore we will consider it the overall area.</i> Therefore, we can use, $A = \pi D_i L$ We isolate L (length of tubes/reactor), Hence $L = \frac{A}{\pi D_i}$ $L = 2\text{m}$	For β_0: $\beta_0 = \frac{G(1-\phi)}{\rho_c g_c D_p^{\frac{5}{2}}} \left[\frac{150(1-\phi)}{D_p} + 1.75G \right]$ We know: $G = 2.7 \times 10^{-3} \frac{\text{kg}}{\text{m}^2 \text{s}}$ $(1-\phi) = .6$ $\rho_c = 1600 \frac{\text{kg}}{\text{m}^3}$ $g_c = 1 \frac{\text{kg m}}{\text{N s}^2}$ $D_p = .005\text{m}$ $\phi^2 = .064$ $\mu = 7.5 \times 10^{-6} \frac{\text{kg}}{\text{m s}}$ Hence, $\beta_0 = \frac{2.7 \times 10^{-3} \frac{\text{kg}}{\text{m}^2 \text{s}} (.6)}{(1600 \frac{\text{kg}}{\text{m}^3}) (1 \frac{\text{kg m}}{\text{N s}^2}) (.005\text{m}) (.064)^{\frac{5}{2}}} \left[\frac{150(.6)}{(.005\text{m})} + 1.75(2.7 \times 10^{-3} \frac{\text{kg}}{\text{m}^2 \text{s}}) \right]$ $\beta_0 = 4.4 \times 10^{-4} \frac{\text{Pa}}{\text{m}}$ For α: $\alpha = \frac{2\beta_0}{A \rho_c (1-\phi) P_0}$ We know: $A = .285\text{m}^2$ $\beta_0 = 4.4 \times 10^{-4} \frac{\text{Pa}}{\text{m}}$ $\rho_c = 1600 \frac{\text{kg}}{\text{m}^3}$ $(1-\phi) = .6$ $P_0 = 1\text{atm} - 160\text{atm}$ Note: $1\text{atm} = 101325\text{Pa}$ Hence, $\alpha = \frac{2(4.4 \times 10^{-4} \frac{\text{Pa}}{\text{m}})}{(.285\text{m}^2)(1600 \frac{\text{kg}}{\text{m}^3})(.6)(101325\text{Pa})}$ $\alpha = 4.5 \times 10^{-12} / \text{kg}$ <i>Note: the value above is at 1Pa, and can Be repeated for different Pressure values as needed.</i>

Table 3

Results/Polymath

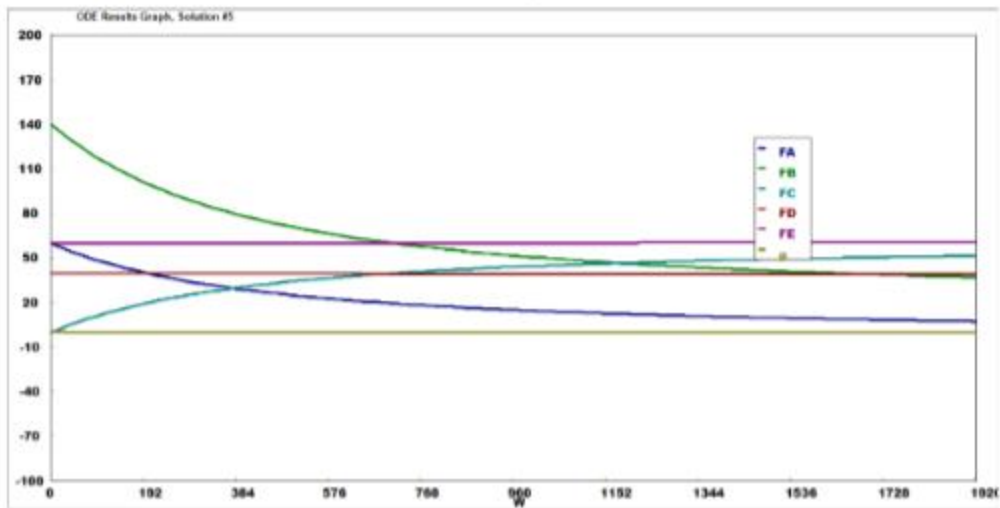


Figure 2: Polymath graph at $P=40$, $T=330$

```

Differential Equations: 6 | Auxiliary Equations: 39 | Ready to solve
# Edgar-Mendoza
# Dynasty-Stephenson
# Jazmans-Carter

# Mole Balance
dFA/dW = rA # CO
dFB/dW = rB # H2
dFC/dW = rC # CH3OH
dFD/dW = rD # H2O
dFE/dW = rE # CO2
FE(0) = 60 # mol/s

FT = FA + FB + FC + FD + FE

# Rate Law
r1 = KPRIME1 * (CA * CB + 2 * CC / K1)
r2 = KPRIME2 * (CA * CD - CE * CB / K2)

# Net Rates
rA = (-r1 - r2)
rB = (-2 * r1) + r2
rC = r1
rD = -r2
rE = r2

KPRIME1 = k1 / pb
KPRIME2 = k2 / pb

# Concentrations
CA = CTO * (FA / FT) * P / Pb
CB = CTO * (FB / FT) * P / Pb
CC = CTO * (FC / FT) * P / Pb
CD = CTO * (FD / FT) * P / Pb
CE = CTO * (FE / FT) * P / Pb

# Given Data
mpo = 5.31 # initial mass flow rate
go = 1 # gravitational constant
vo = FTO / CTO # initial volumetric flow rate m³/s
Pb = 60 # Can vary as needed
po = 1600 # gas density (kg/m³)
R = 1.987
CTO = Pb / ((8.2057 * 10⁻⁵) * T)
pb = 960 # bulk density
pc = 1600 # catalyst density
O = 0.4 # void fraction
id = 0.0201 # inner diameter (m)
od = 0.042 # outer diameter (m)
n = 250 # Number of tubes in reactor for design
k1 = (0.933 * 10⁻⁵) * exp(2.5 * ((31400 / R) * ((1 / 330) - (1 / T))))
k2 = (0.636 * 10⁻⁵) * exp(18000 / R) * ((1 / 300) - (1 / T))
K1 = (131657 * ((0.001987 * T)²) * exp(30620 / R) * ((1 / T) - (1 / 298)))
K2 = (103942) * exp(9634 / R) * ((1 / T) - (1 / 298))
Pb = 4.4 * 10⁻⁴ # (Pa/m)
A = 3.17E-11 # unit (1/kg) at 1Pa
dp/dW = -(Bb / Ac * (1 - O) * pc * (T / To) * (FT / FTO) * p
p(0) = 1
Ac = n * 3.14 * (id² / 4) # Cross sectional area of reactor
To = 330 # initial temperature entering the reactor (K)
P = 60
T = 330
FTO = 300

```

Figure 3: Polymath Code

Inlet Temperature (K)	330
Outlet Temperature (K)	360
Inlet Pressure (Pa)	40
Outlet Pressure (Pa)	60
Maximum tube-side Temperature (K)	375
Methanol production rate (Kg/s)	0.6
Reactor Length (m)	2.0
Total inlet concentration at 330K	1477.17
Rate Constant, k_1 at 330K	9.33×10^{-3}
Equilibrium constant K_C , 1 at 330K	375.95
Rate constant, k_2 at 330K	9.9×10^{-6}
Equilibrium constant K_C , 2 at 330K	20770
Heat of reaction for reaction 1 at 330k	-48.98
Heat of reaction for reaction 2 at 330K	-19.51
Stoichiometric feed H_2 to CO	2:1
Stoichiometric feed H_2O to Co	1:1
heat transfer coefficient, U (W/m ² *K)	631

Table 4: Reactor Data 1

Table name and number goes on top of the table

Side Note: After doing our calculations and typing in the algorithm, we concluded that our optimum pressure is 40 atm (4053000 Pa) and

	In Reactor	Out Reactor
Flow (mol.s-1)	300	183.9
Pressure (Pa)	40	60
Temperature (K)	330	330
CO (mole fraction)	0.2	0
H2 (mole fraction)	0.47	0.24
CO2 (mole fraction)	0.2	0.05
CH3OH (mole fraction)	0	0.71
H2O (mole fraction)	0.13	0

Table 5: Reactor Data 2

Discussion/ Task 1

The economic feasibility of methanol synthesis as a method for CO₂ reduction and energy storage has been an analysis that has been studied to evaluate how to obtain methanol from the chemical reaction. Some studies paid attention to the design and modeling of methanol synthesis process, others focused on the electrolysis technology, and implementation in a future renewable-based energy system. Greenhouse gas is used in energy supply, industry, agriculture, etc. and according to our research approximately 36.44 billion of total global CO₂ emission from fuel combustion. Research shows that greenhouse gases has been a problem for centuries and serves as a climate control for the earth. As technology has improved there has been an increase of CO₂ emissions and there have been efforts towards trying to regulate it. Through time greenhouse gas emissions must be reduced because of major effects of global climate change, flooding, and desertification. Comparisons of methanol, from recycled CO₂, emitted from a fossil-fuel power station to hydrogen produced by water electrolysis. There are three types of electrolysis, alkaline water electrolysis polymer electrolyte/proton exchange membrane water and solid oxide high temperature electrolysis. With these three electrolysis technologies for

green H_2 production method for the making of methanol. Our catalyst chosen for our reactor, Cu/ZnO, would speed up the rate of the reaction which would save money because the process wouldn't have to operate for as long to get the same amount of product. The catalyst would reduce the amount of energy which is good for sustainable development used in the reaction. Also taking into consideration, methanol electrical energy prices, the different oxygen selling prices, and PEM electrolyze capital cost. MeOH is a renewable energy-based electricity. To make methanol using CO_2 hydrogenation, the process needs minimum production cost and can sustain the operating conditions as well. Most of the energy that is produced in the world is mainly from combustion.

The production of methanol is majorly important as it is used as a feedstock for production of other chemicals; natural gas, biomass or coal is used as the feedstock. Carbon dioxide (CO_2) mitigates CO_2 emissions to the atmosphere is converting CO_2 to a valuable product resulting in methanol. This study shows the application of response surface methodology for optimization methanol production using CO_2 hydrogenation. Methanol production process starts as gasification of any solid bearing such as biomass or reforming of natural gas to produce carbon monoxide, carbon dioxide, and hydrogen which is used eventually in the process to produce methanol over Cu- based catalyst. According to the chemical industry, the downstream of methanol purification stage to specifications from costumers. The overview of methanol production process: (1) reaction of carbon monoxide with hydrogen (2) reaction of carbon dioxide with hydrogen (3) water-gas shift reaction (4) have a stoichiometric ratio of 2:1. The three main concepts to remember for this process: gasification of carbon to produce syngas (mixture of carbon monoxide and hydrogen, methanol synthesis and product upgrading. For the syngas phase, natural gas is used for the raw material due to low sulphur content and undesirable purities. Coal is the second largest used for the syngas used to produce methanol. The process can achieve a high conversion and quality by selecting a suitable coal gasifiers, reactors, and process equipment and optimal pressure and temperatures. Methanol synthesis favors optimum temperatures and high pressures. The ratio 2:1 is the efficiency produced for methanol and we know that any stoichiometric number larger than 2 is optimal for majority of catalyst. Water-gas shift (WGS) is an important step in methanol synthesis because it adjusts the CO_2 and H_2 ratio during the syngas phase.

According to Radhi, the net of CO_2 would increase 5.4% over the next few decades. Hydrogenation of carbon monoxide and carbon dioxide is reversible and exothermic. Operating the reactor at a low temperature would require a large amount of catalyst due to the low reaction rate. Due to this reasoning, the optimal temperature profile along reaction would ensure high methanol yield with a good reasonable amount of catalyst. By cooling the reaction mixture would be achieved by using a temperature profile close to the optimum temperature. One reactor type would be an **adiabatic multibed reactor with (indirect) external cooling**. With this reactor type all the gas passes through the first adiabatic bed. The gas exits from the first bed and then enters the first heat exchanger. Next, the mixture cools and the heat available is used for steam generation. On the other hand, with the direct cooling reactor, the volume of the catalyst is smaller due to the gas going through the catalyst. The reaction rate would still be away from the maximum reaction rate curve. The downfall of the reactor type is it needs to operate high-

pressure unit such as catalyst with several catalyst beds, heat exchangers, etc. Due to this it would have a higher capital cost. Below showcases the configuration of adiabatic reactor for indirect external cooling showing the inlet temperatures. There would be higher efficiency if there were lower inlet temperatures, but it would require more catalyst. Another reactor we can use for methanol synthesis, **Adiabatic multibed reactor with quench (direct) cooling**. Unlike the adiabatic reactor with indirect cooling, this reactor requires a larger catalyst volume as the catalyst is not fully utilized because the reactants are fed at different points in the reactor. The configuration below shows the yield dropping as the reactants enter at different points. This process has many variables to control and is complex to optimize. The largest capacity is estimated to be 3000-3500 t/day because of manufacturing limitations. This process is a high-pressure vessel with an increase of pressure drop throughout the catalyst beds which causes power to recirculate those results in energy consumption. The first catalyst bed inlet splits the feed stream and that's determined by the amount of catalyst needed to achieve the required productivity. Compared to the adiabatic reactor with indirect cooling this reactor would have a lower conversion, but the use of heat exchangers is eliminated which would equvalate to a much lower investment cost.

Given the condition in the problem statement for our shell-and- tube packed bed reactor, we decided the best catalyst to use is Cu/ZnO. In 1960, Cu/ZnO-based catalyst were developed by a co-precipitation method. This discover advanced methanol synthesis because it increased the amount of methanol that can be created through the synthesis process. Cu/ZnO catalyst is the most commercial use for methanol synthesis from carbon dioxide hydrogenation. Cu/ZnO is a metallic copper-based catalyst consisting of 50% aluminum and 50% copper-zinc mixture. This catalyst is most active between temperatures 473.15K and 573.15K and pressures 50atm and 100atm. In recent years scientist has been observing different properties of this catalyst including surface area and particle size. It was found that the selectivity of methanol was highest when it was fine particles, ration of copper to zinc was 1, and large surface area. Currently Chemical engineers are still looking at different catalyst that can be used to make the process of methanol synthesis more efficient but as in today Cu/ZnO is the commercial choice. The process of methanol synthesis is a reaction process including hydrogenation reaction that produces methanol, next it would be another hydrogenation reaction that produces methanol and water, and lastly carbon monoxide reacts with water to produce carbon dioxide and hydrogen gas. Through these reactions to create methanol some methanol is being lost in the conversions. Using the catalyst Cu/ZnO/Al₂O₃ many challenges has been faced with making the synthesis process more efficient to be able to create as much methanol as possible. The problem occurs in the second reaction when CO₂ is being converted to methanol directly. In this reaction a low single pass conversion, high pressure, and low methanol selectivity occurs.

As of today, scientist is looking for ways to make this process more efficient. Global warming is caused by many things happening to the atmosphere but today 2/3 of the energy balanced that is causing Earth's temperature to rise is because of the amount of in the atmosphere. Today around 500 liters of enters the earth atmosphere everyday having a total of .04% of the air being. Methanol is something that can not only help with our global warming problem but help the world. Methanol, also known as methyl alcohol, is a highly versatile

chemical widely used for industrial purposes and prevalent in our everyday life. A few products it can be used for plastics, paints, car parts, fuel cells, boilers, cook stoves, even a clean energy resource to fuel cars, trucks, ships, and so much more. Today the main way to synthesis methanol is from consumption. The use of these two compounds makes Methanol the perfect alternative renewable energy source. With the popularity of methanol, the methanol industry has been a great benefit for global economy generating over \$12 billion in annual economic activity while creating over 100,000 direct and indirect jobs.

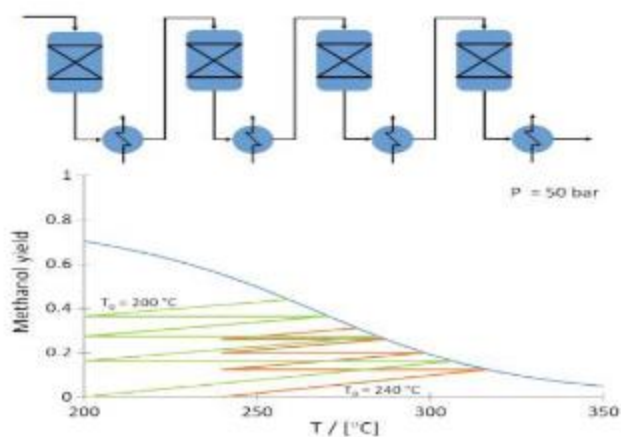


Figure 4: Adiabatic Multibed Reactor with Indirect (External) Cooling Configuration

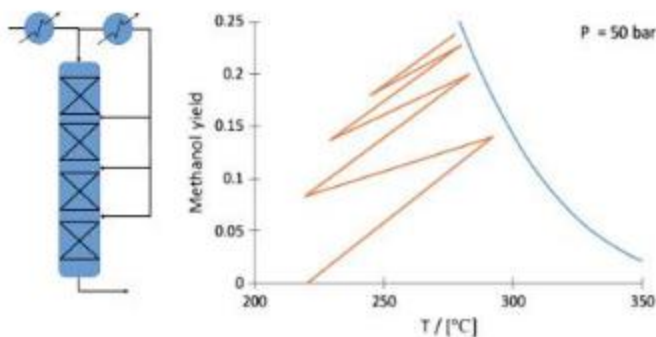


Figure 5: Adiabatic Multibed Reactor with quench (Direct) Cooling Configuration

Reflection/Conclusion

In conclusion, we were asked to design a shell and tube packed-bed reactor for methanol synthesis. As a group, we were able to stick to our original plan from start to finish by breaking down the problem given, successfully using Polymath, and discovering useful research. The group evenly distributed the work amongst one another by assigning task of typing and calculating. With our group successfully able to complete our certain task there wouldn't be another approach to go about the project. This project was very informative with learning about methanol synthesis with intense research and analyzing the chemical reaction given to us. We've had multiple meetings amongst ourselves and the professor and made improvements with our calculations, correct formulas, clarifications with the rubric, and schematic. On pages 5-7 shows our givens, algorithm steps, and determining our missing variables. We developed graphical representation of each molecular flow rate for the components as a function of catalyst weight in Polymath. This project did help with our time management, problem-solving, and overall teamwork contribution from each team member. It was a great learning experience and will be useful for senior design in the upcoming future.

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Methanol Synthesis

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Erron Williams
Oluwatuminu Alade



Presentation Topics: Outline

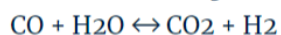
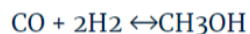


1	Problem Statement	✓ Design a reactor for methanol synthesis	7	Algorithm	✓ Mole Balance, Rate Law... ✓ Isothermal, Isobaric ✓ Pressure Drop
2	Introduction	✓ Methanol Synthesis ✓ Objectives (Tasks) ✓ Packed Bed Reactor	8	Polymath Codes	✓ Code 1: Isothermal, Isobaric ✓ Code 2: Pressure drop
3	Project Objectives	✓ Given Tasks/ Instructions	9	Results	✓ Graphs ✓ Tabular Data
4	Reactor Design	✓ Packed Bed Reactor ✓ Assumptions	10	Discussion	✓ Polymath ✓ Catalyst Research
5	Methods & Calculations	✓ Equations Used ✓ Concepts	11	Conclusion	✓ Optimal Conditions of the Reactor & Supporting data
6	Catalyst Selection	✓ Copper Based Catalyst	12	References	



Problem Statement

A new catalyst has been proposed for the synthesis of methanol from carbon monoxide and hydrogen gas. This catalyst is reasonably active between temperatures of 330 K to about 400K. The reactions to be considered are:



The reactions are elementary and occur in a reactor containing tubes packed with a precious metal catalyst on a silica support. Heat is removed from the reactor by generating steam on the shell side of the tubes. The feed consists of 7/15 hydrogen gas, 1/5 carbon monoxide, 1/5 carbon dioxide, and 2/15 steam. The total flow rate is 300 mol.s^{-1} . The entering pressure may vary between 1 atm and 160 atm and the entering temperature is between 300K and 400K. A total tubular reactor volume of 2 m^3 is to be used.

3

Introduction

1

Objectives



Task 1: Commercial Applications, economics, process conditions, reactor types and configurations typically used, catalyst types, and end product usage



Task 2: Assuming isothermal and isobaric conditions, determine the entering conditions of temperature and pressure that will optimize the production of methanol. Hint: Do this by conducting several simulations at discrete combinations of T_0 and P_0 . First try $T_0 = 330$ at $P_0 = 40$ atm, then try $T_0 = 380$ and $P_0 = 1$ atm)



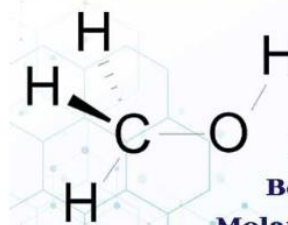
Task 3: Carry out a detailed reactor design of a shell and tube reactor for the optimal feed conditions determined from part 2.



What is Methanol?

- ❑ Non-consumable form of alcohol
- ❑ High carbon to hydrogen ratio
- ❑ Good source of energy or fuel

Methanol(CH_3OH)



Formula: CH_3OH

Density: 792 kg/m^3

Boiling point: 64.7°C

Molar mass: 32.04 g/mol

Melting point: -97.6°C

Vapor pressure: 13.02 kPa

Methanol Background

Common Applications

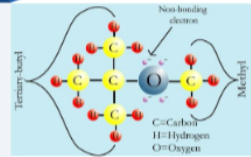
- Produce (MTBE) component in gasoline that reduces carbon emissions
- Produce (DME) Dimethyl- Ether which is a clean burning fuel

1

2

Economics

Methanol Costs: .60¢/ gal



Uses

- Plastics
- Construction materials
- Paints
- Car parts
- Energy or fuel

3

4

Multi-tubular Fixed Bed reactor

Packed Bed Reactors

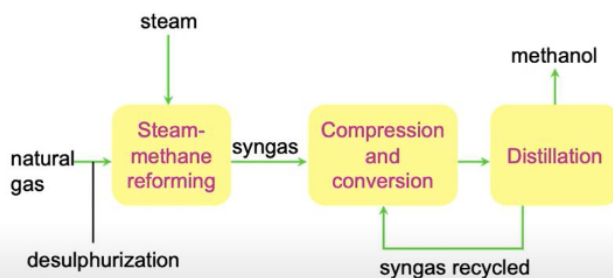
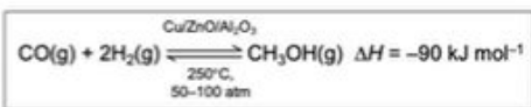
Common types of Reactors

Dimethyl ether



Atomic weight	Number of atoms		Molecular Weight
12.0107	2	$12.0107 \times 2 = 24.0214$	46.0688
1.008	6	$1.008 \times 6 = 6.048$	
15.9994	1	$15.9994 \times 1 = 15.9994$	

How is Methanol Made?



- Sulfur and impurities are removed from Natural gas at the inlet.
- Metgas (Steam) is added to the purified natural gas and forms syngas (Synthetic gas)
- The Syngas is compressed and converted.
- Methanol is converted from syngas by using a catalyst (in this case a copper based catalyst).

Which Catalyst? Why?

The Cu/ZnO/Al₂O₃ catalyst is the best catalyst for the synthesis of Methanol.

Pros:

- ❑ Cu/ZnO/Al₂O₃ is capable of catalyzing at low temperatures.
- ❑ If the temperature of the catalyst is increased then the catalyst can be accelerated within.

Cons:

- ❑ The copper nanoparticles are prone to sintering (turns into a solid)

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Kinds of Reactors for Methanol Synthesis

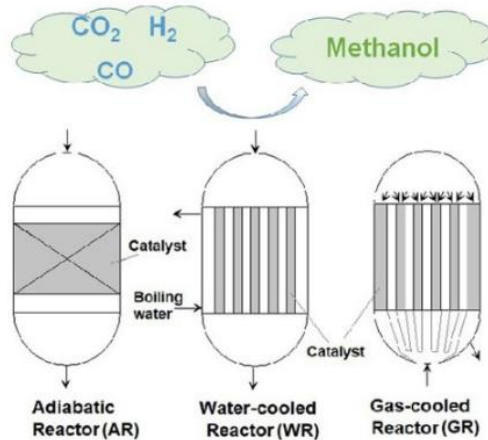
Adiabatic Reactor: *The temperature increase in each catalyst bed is attributed to the exothermic reactions*

Gas Cooled Reactor:

In this reactor, the catalyst bed is in the shell side and cooled by the cold feed in the tube side

Water Cooled Reactor:

The water-cooled reactor or boiling water reactor with a shell-tube structure is widely used for methanol production



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Reactor Design

Reactor dimensions:

Reactor equipment data:

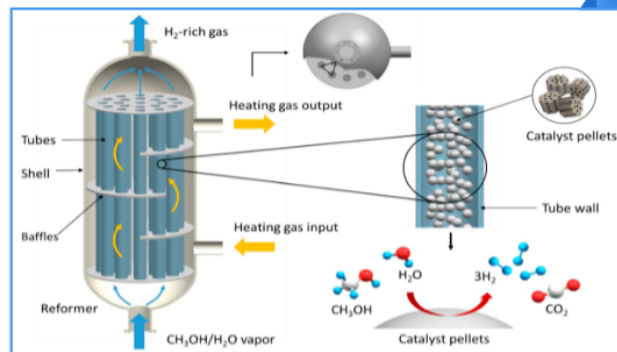
- Catalyst bed void fraction: 40%
- Catalyst density: 1600 kg.m^{-3}
- Tube diameter (i.d.): 3.81 cm
- Overall heat transfer coefficient: $631 \text{ W.m}^{-1} \text{ .K}^{-1}$
- Tube diameter (o.d.): 4.20 cm = 0.042m
- Shell side water temperature: 373 K
- Catalyst particle size: 5mm
- Average gas viscosity, assumed constant over all temperature: $7.5 \times 10^{-6} \text{ Pa.s}$
- Number of tubes in the heat exchanger: 250 tubes

Temp range = 300K to 400K

$R = 1.987 \text{ cal.mol}^{-1} \text{ .K}^{-1}$

Pressure range = 1atm and 160atm

Reactor Volume = 2 m^3



Phases Involved	Usage	Advantages	Disadvantages
Gas-Phase/solid catalyzed	Heterogeneous Reactions w/ catalyst	High conversion per unit mass of catalyst	Poor temp. control
Gas-solid reactions			Channeling It May be difficult to clean

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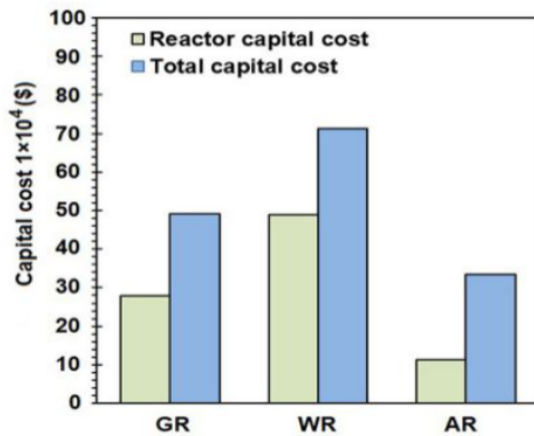
Safety

In order to take into account safety we considered the problems statement values for our safety bounds. 330-380K, 1-40 Atm

Note: Since Isothermal conditions were assumed, a real world application of this process would need to analyze Feed-Temp Relationship.

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Costs of Each Reactor?



The water gas reactor shows the highest reactor capital costs.

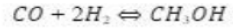
The capital costs of the water gas reactor has a larger tube diameter and reactor diameters.

The adiabatic reactors with the lowest cost

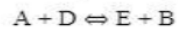
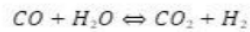
13

Methods And Calculations

Equation 1:



Equation 2:



Mole Balance:

$$\frac{dF_A}{dW} = r'_A$$

$$\frac{dF_B}{dW} = r'_B$$

$$\frac{dF_C}{dW} = r'_C$$

$$\frac{dF_D}{dW} = r'_D$$

$$\frac{dF_E}{dW} = r'_E$$

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Algorithm Cont.d

Rate laws:

The rate laws are as follows:

$$r_{A1} = -K_1 C_A C_B^2$$

$$r_{A2} = -K_2 C_A C_D$$

Net rate:

$$r_A = r_{A\text{net}} = r_{A1} + r_{A2}$$

$$r_B = r_{B\text{net}} = -K_1 C_A C_B^2 + K_2 C_A C_D$$

$$r_D = K_2 C_A C_D$$

Relative rates:

For equation 1:

$$-r_{A1} = \frac{r_B}{-2} = r_C$$

For equation 2:

$$-r_{A2} = -r_D = r_E = r_B$$

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Algorithms cont.d

Stoichiometry:

$$C_A = C_{TO} \left(\frac{F_A}{F_T} \right) \cdot \frac{p}{p_0}$$

$$C_B = C_{TO} \left(\frac{F_B}{F_T} \right) \cdot \frac{p}{p_0}$$

$$C_C = C_{TO} \left(\frac{F_C}{F_T} \right) \cdot \frac{p}{p_0}$$

$$C_D = C_{TO} \left(\frac{F_D}{F_T} \right) \cdot \frac{p}{p_0}$$

$$C_E = C_{TO} \left(\frac{F_E}{F_T} \right) \cdot \frac{p}{p_0}$$

do not copy write the equations clearly -2

Where: $p = \frac{P}{P_0}$ represents pressure drop.

$$\text{Also, } F_T = F_A + F_B + F_C + F_D + F_E$$

16

Algorithms cont.d

Stoichiometry:

$$C_A = C_{TO} \left(\frac{F_A}{F_T} \right) \cdot \frac{P}{P_0}$$

$$C_B = C_{TO} \left(\frac{F_B}{F_T} \right) \cdot \frac{P}{P_0}$$

$$C_C = C_{TO} \left(\frac{F_C}{F_T} \right) \cdot \frac{P}{P_0}$$

$$C_D = C_{TO} \left(\frac{F_D}{F_T} \right) \cdot \frac{P}{P_0}$$

$$C_E = C_{TO} \left(\frac{F_E}{F_T} \right) \cdot \frac{P}{P_0}$$

do not copy write the equations clearly -2

Where: $p = \frac{P}{P_0}$ represents pressure drop.

$$\text{Also, } F_T = F_A + F_B + F_C + F_D + F_E$$

16

Algorithms Cont.

$$A = \frac{\pi d^2}{4} N_r$$

$$A = \frac{3.142 \cdot 0.0381^2 \cdot 250}{4} = 0.29 \text{ m}^2$$

$$\text{length, } z = \frac{V}{A} = \frac{2 \text{ m}^3}{0.29 \text{ m}^2} = 7.02 \text{ m}$$

Weight of catalyst, W

$$W = A \rho (1-\phi) z$$

$$W = 0.29 \times 1600(1-0.4) \times 7.02 = 1920 \text{ kg}$$

Mass velocity, G

$$G = \rho \mu = \frac{m}{A}$$

$$G = \frac{4.6}{0.29}$$

$$G = 15.86 \text{ kg/m}^2 \text{ s}$$

$$\beta_o = \frac{G(1-\phi)}{g_c \rho_o D_p \phi^3} \left[\frac{150(1-\phi)\mu}{D_p} + 1.75G \right]$$

$$= \frac{15.86(1-0.4)}{1.25 \cdot 56 \cdot 0.0381 \cdot 0.4^3} \left[\frac{150(1-0.4)7.5 \cdot 10^{-6}}{0.0381} + 1.75(15.86) \right]$$

$$\beta_o$$

$$= 4240.4 \frac{\text{Pa}}{\text{m}}$$

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Polymath Code

```

# CHEG 3306 Final Project
# Objective 1
# Group 1
# Janera Perry
# Oluwatunmbi Alade
# Eron Williams
# Dr. Nabila Shamim

# Conditions
T = 330 # 1st simulation Initial Temperature entering reactor [K]
P = 40 # 1st Simulation Initial Pressure entering reactor [atm]
Fto = 300 # Total initial molar flow rate [mol/s]
R = 1.987 # Gas constant [cal/mol*K]
Po = 40 # Assuming isobaric
To = 330 # Assuming Isothermal

# Reactor Equipment Data:
cbf = 0.40 # Catalyst bed void fraction
pc = 1600 # Catalyst density [kg/m^3]
di = 0.0381 # Tube inner diameter [m]
do = 0.042 # Tube out diameter [m]
U = 631 # Overall heat transfer coefficient [W m^-1 K^-1]
Dp = 0.005 # Catalyst particle size [m]
Vsc = 7.6 * 10^-6 # Average gas viscosity [Pa.s]
Nth = 250 # Number of tubes in heat exchanger

# Constants
K1 = (131667 * ((0.001987 * T) ^ 2)) * exp((30620 / R) * ((1 / T) - (1 / 298))) # [dm^6/s*mol^2]
K2 = (103943 * exp(9834 / R) * ((1 / T) - (1 / 298))) # [dm^3/mol]
k1 = (0.933 * 10^-6) * exp(2.5 * ((31400 / R) * (1 / 330) - (1 / T))) # [dm^6/s*mol^2]
k2 = (0.636 * 10^-6) * exp((18000 / R) * ((1 / 300) - (1 / T))) # [dm^3/mol]

# Mole Balance Values
Fco2(0) = 60
W(0) = 0
W(t) = 1920
Fh2(0) = 140
Fco(0) = 60
Fch3oh(0) = 0
Fh2o(0) = 40

# Mole balances
d(Fh2)/d(W) = rh2 # hydrogen
d(Fco)/d(W) = rco # Carbon monoxide
d(Fch3oh)/d(W) = rch3oh # Methanol
d(Fh2o)/d(W) = rh2o # Water
d(Fco2)/d(W) = rco2 # Carbon Dioxide

# Auxiliary Calculations
mo = 4.6 # Total initial mass flow rate [kg/s]
Ac = Nth * 3.14 * (di ^ 2 / 4) # Cross sectional area of reactor
Cto = Po / ((8.2057 * 10^-5) * To) # Initial concentration [mol/m^3]
vo = Fto / Cto # Initial volumetric flow rate [m^3/s]
G = mo / Ac # Superficial mass velocity [kg/m^2*s]
po = mo / vo # Initial density [kg/m^3]
gc = 1 # gravitational constant
Bo = G * (1 - cbf) / (po * gc * Dp * cbf ^ 3) * (150 * (1 - cbf) * Vsc / Dp + 1.75 * G) # Constant based on packed bed [Pa/m]
alpha = (3.18 * 10^-4)
pb = (1 - cbf) * pc
kprime1 = k1 / pb
kprime2 = k2 / pb

# Concentrations in [mol/dm^3]
Cco = Cto * (Fco / Ft) * (P / Po) * (To / T)
Cco2 = Cto * (Fco2 / Ft) * (P / Po) * (To / T)
Ch2 = Cto * (Fh2 / Ft) * (P / Po) * (To / T)
Ch2o = Cto * (Fh2o / Ft) * (P / Po) * (To / T)
Cch3oh = Cto * (Fch3oh / Ft) * (P / Po) * (To / T)

S = Cch3oh / (Ch2o + Cco) # Selectivity

Ft = Fco + Fco2 + Fh2 + Fh2o + Fch3oh # Total Molar flow rate
    
```

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Polymath Code cont.

```

# CHEG 3306 Final Project
# Objective 3-1
# Group 1
# Janera Perry
# Oluwatunmbi Alade
# Eron Williams
# Dr. Nabila Shamim

# Conditions
T = 330 # 1st simulation Initial Temperature entering reactor [K]
P = p # Po # Pressure in relation to pressure drop
Fto = 300 # Total initial molar flow rate [mol/s]
R = 1.987 # Gas constant [cal/mol*K]
Po = 40 # 1st Simulation Initial Pressure entering reactor [atm]
To = 330 # Assuming Isothermal

# Pressure Drop
dp/d(W) = -alpha / (2 * pi) * (T / To) * (Ft / Ft0)
p(0) = 1

# CHEG 3306 Final Project
# Objective 3-2
# Group 1
# Janera Perry
# Oluwatunmbi Alade
# Eron Williams
# Dr. Nabila Shamim

# Conditions
T = 380 # 2nd simulation Initial Temperature entering reactor [K]
P = p # Po # Pressure in relation to pressure drop
Fto = 300 # Total initial molar flow rate [mol/s]
R = 1.987 # Gas constant [cal/mol*K]
Po = 1 # 2nd Simulation Initial Pressure entering reactor [atm]
To = 380 # Assuming Isothermal

# Pressure Drop
dp/d(W) = -alpha / (2 * pi) * (T / To) * (Ft / Ft0)
p(0) = 1
    
```

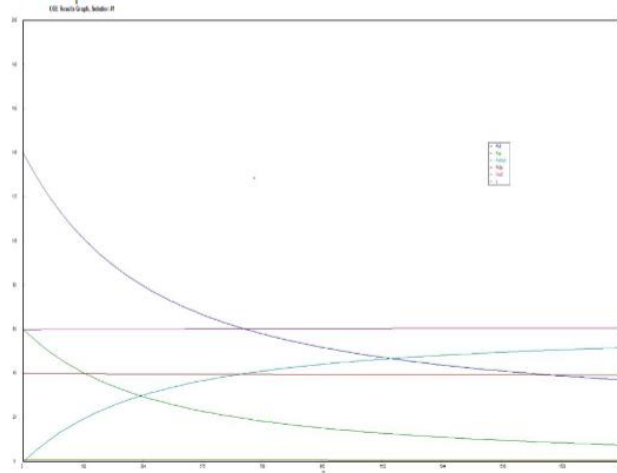
20

Results

Table 1

Variable	Initial value	Minimal value	Maximal value	Final value
1 W	0	0	1920.	1920.
2 Fh2	140.	37.23005	140.	37.23005
3 Fco	60.	7.650318	60.	7.650318
4 Fch3oh	0	0	51.70654	51.70654
5 Fh2o	40.	39.35606	40.	39.35606
6 Fco2	60.	60.	60.64314	60.64314
7 p	1.	0.7417648	1.	0.7417648
8 chvf	0.4	0.4	0.4	0.4
9 pc	1600.	1600.	1600.	1600.
10 di	0.0381	0.0381	0.0381	0.0381
11 do	0.042	0.042	0.042	0.042
12 U	631.	631.	631.	631.
13 Do	0.005	0.005	0.005	0.005
14 Vsc	7.6E-06	7.6E-06	7.6E-06	7.6E-06
15 Nth	250.	250.	250.	250.
16 ntr	150.	150.	150.	150.
17 Pto	300.	300.	300.	300.
18 R	1.987	1.987	1.987	1.987
19 Po	40.	40.	40.	40.
20 To	330.	330.	330.	330.
21 mo	4.6	4.6	4.6	4.6
22 Ac	0.2848785	0.2848785	0.2848785	0.2848785
23 Cto	1477.17	1477.17	1477.17	1477.17
24 va	0.2030911	0.2030911	0.2030911	0.2030911
25 G	16.14724	16.14724	16.14724	16.14724
26 po	22.64994	22.64994	22.64994	22.64994
27 gc	1.	1.	1.	1.
28 Bo	3.795E+04	3.795E+04	3.795E+04	3.795E+04
29 alpha	0.000318	0.000318	0.000318	0.000318
30 pb	960.	960.	960.	960.
31 T	330.	330.	330.	330.
32 P	40.	40.	40.	40.
33 Ft	300.	196.5869	300.	196.5869
34 Cco	295.434	37.4801	295.434	37.4801
35 Cco2	295.434	295.434	455.6774	455.6774
36 Ch2	689.3459	279.7496	689.3459	279.7496
37 Ch2o	196.956	196.956	295.7306	295.7306
38 k1	9.33E-07	9.33E-07	9.33E-07	9.33E-07

Graph 1



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Results cont.d

Table 2

Variable	Initial value	Minimal value	Maximal value	Final value
1 W	0	0	1920.	1920.
2 Fh2	140.	25.5073	140.	25.51127
3 Fco	60.	2.751748	60.	2.751748
4 Fch3oh	0	0	57.24669	57.24566
5 Fh2o	40.	39.99741	40.	39.99741
6 Fco2	60.	60.	60.00259	60.00259
7 p	1.	0.7881112	1.	0.7881112
8 chvf	0.4	0.4	0.4	0.4
9 pc	1600.	1600.	1600.	1600.
10 di	0.0381	0.0381	0.0381	0.0381
11 do	0.042	0.042	0.042	0.042
12 U	631.	631.	631.	631.
13 Do	0.005	0.005	0.005	0.005
14 Vsc	7.6E-06	7.6E-06	7.6E-06	7.6E-06
15 Nth	250.	250.	250.	250.
16 ntr	150.	150.	150.	150.
17 Pto	300.	300.	300.	300.
18 R	1.987	1.987	1.987	1.987
19 Po	1.	1.	1.	1.
20 To	380.	380.	380.	380.
21 mo	4.6	4.6	4.6	4.6
22 Ac	0.2848785	0.2848785	0.2848785	0.2848785
23 Cto	32.07013	32.07013	32.07013	32.07013
24 va	9.354498	9.354498	9.354498	9.354498
25 G	16.14724	16.14724	16.14724	16.14724
26 po	0.491742	0.491742	0.491742	0.491742
27 gc	1.	1.	1.	1.
28 Bo	1.748E+06	1.748E+06	1.748E+06	1.748E+06
29 alpha	0.000318	0.000318	0.000318	0.000318
30 pb	960.	960.	960.	960.
31 T	380.	380.	380.	380.
32 P	1.	1.	1.	1.
33 Ft	300.	185.5066	300.	185.5067
34 Cco	6.414027	0.4757131	6.414027	0.4757131
35 Cco2	6.414027	10.37305	10.37305	10.37305
36 Ch2	14.96606	4.409668	14.96606	4.410305
37 Ch2o	4.276018	4.276018	6.915033	6.914621

Graph 2



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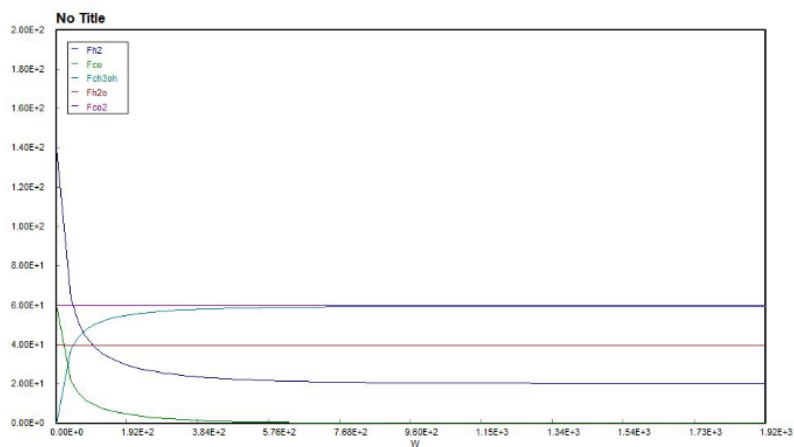
Results (Optimal Conditions)

Temperature	Pressure	Selectivity
330	40	1.10
380	1	1.34
390	1	1.20
370	1	1.40
360	1	0.52
371	1	1.41
371	5	1.495
371	20	1.4997
371	40	1.49986

Temperature	Pressure	Selectivity
369	40	1.49988
365	40	1.49992
350	40	1.50007
340	40	1.50106
335	40	1.47650
339	40	1.50135
337	40	1.49994
338	40	1.50143

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Results (Graph)



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Discussion

- ▶ Trial & Error Method used to find the highest selectivity for Optimal Conditions
- ▶ Pressure and Selectivity are directly proportional
- ▶ Optimal Temperature Varied at different pressures
- ▶ Pressure Drop decreased selectivity of trials by a range of (4-15%)

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Conclusion

This project consisted of the methods necessary to design a packed bed reactor used for methanol synthesis.

The materials used to evaluate the necessary design criteria mainly consisted of trial and error using the polymath coding software. The second task within the problem statements required that the reactor operate under isothermal and isobaric conditions.

These conditions are much easier to evaluate using the polymath software since most of the assumptions allowed for less calculation.

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References

“Energies | Free Full-Text | Modeling and Design of a Multi-Tubular Packed-Bed Reactor for Methanol Steam Reforming over a Cu/ZnO/Al₂O₃ Catalyst.” *MDPI*, Multidisciplinary Digital Publishing Institute, <https://www.mdpi.com/1996-1073/13/3/610>. Accessed 6 May 2022.

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AVERAGE

Average Student Original Graded Assignment

Prairie View A&M University

Roy. G. Perry College of Engineering



CHEMICAL REACTION ENGINEERING

CHEG 3306 FINAL PROJECT

Submitted by: Janeria Perry, Oluwatumininu Alade, Erron Williams

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Executive Summary

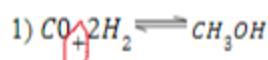
Methanol Synthesis Synopsis:

Methanol is frequently used as an energy source that is derived from renewable resources. The chemical formula of Methanol is (CH₃OH) and it is a colorless, volatile, and flammable liquid. Methanol is produced by the hydrogenation of carbon monoxide/carbon dioxide at relatively high temperatures and pressures using copper-based catalysts. To efficiently synthesize methanol the selection of a good catalyst is necessary; an ideal catalyst would be one that produces a high amount of carbon monoxide conversion and a significant amount of selectivity of methanol. Hydrogenation reactions are exothermic and require specific temperature and pressure manipulation. The high reaction temperatures will cause the thermodynamic equilibrium constant (k) to decrease as the temperature increases, as they are inversely related. Packed Bed reactors are the most common type of reactor used to synthesize methanol; the same reactor will be used for this report. An overall analysis of methanol synthesis will require an understanding of heat transfer, energy transfer, and mass transfer.

Introduction:

There are several economical uses of methanol. Methanol is commonly produced for fuel production in vehicles and ships; and is found in everyday products such as paint, plastics, and adhesives. There is an increasing demand for the development of sustainable methanol synthesis. The general process of the heterogeneous catalytic hydrogenation of CO₂ to methanol will be used to describe methanol synthesis at a base level.

The first reaction involved in methanol synthesis:



The combination of carbon monoxide and hydrogen gas is referred to as metgas (derived from steam reforming of fossil fuels). This met gas is passed over a copper-based catalyst (Cu/ZnO/Al₂O₃) at high pressure (5-10Mpa) between the temperatures (473K-573K). This reaction is exothermic and releases heat which causes a negative enthalpy.

The second equation is the reaction in which methanol is synthesized from CO₂; this reaction is less exothermic and includes a secondary reaction (reaction 3).



The generation of methanol is usually through the hydrogenation of CO₂ contained in syngas. The differences in the synthesis of methanol from pure CO₂ or syngas is

determined by the differences in exothermicity of both processes. The types of catalysts that are best used to produce methanol efficiently are discussed later in this report. The compositions and chemical properties of the catalyst can create different conversion amounts of methanol.

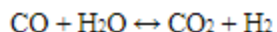
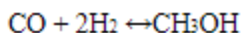
1.1 PROJECT OBJECTIVES:

1. Discuss the commercial application of this reaction in terms of the overall process, economics, process conditions, reactor types and configurations typically used, type of catalyst, typical conversion and end-product usage.
2. Assuming isothermal and isobaric conditions, determine the entering conditions of temperature and pressure that will optimize the production of methanol. Hint: Do this by conducting several simulations at discrete combinations of T_0 and P_0 . First try $T_0 = 330$ at $P_0 = 40$ atm, then try $T_0 = 380$ and $P_0 = 1$ atm)
3. Carry out a detailed reactor design of a shell and tube reactor for the optimal feed conditions determined in part 2. Pressure drop and non-isothermal effects are to be taken into account. The shell side temperature can be controlled by adjusting the steam pressure and maybe assumed constant at a value specified by you. Physical property estimation sources, techniques, and assumptions should be clearly presented. The design should include the following:
 - the reactor dimensions and a number of tubes
 - the reactor conditions; including composition, pressure, and temperature profiles (as a function of reactor length).
 - A mechanical sketch of the reactor should be included.
4. Determine the effect of variations in:
 - ratio of feed H_2 to CO ,
 - ratio of feed H_2O to CO ,
 - assumed heat transfer coefficient, U

1.2 PROBLEM STATEMENT:

A new catalyst has been proposed for the synthesis of methanol from carbon monoxide and hydrogen gas. This catalyst is reasonably active between temperatures of 330 K to about 400K.

The reactions to be considered are:



The reactions are elementary and occur in a reactor containing tubes packed with a precious metal catalyst on a silica support. Heat is removed from the reactor by generating steam on the shell side of the tubes. The feed consists of 7/15 hydrogen gas, 1/5 carbon monoxide, 1/5 carbon dioxide, and 2/15 steam. The total flow rate is 300 mol.s^{-1} . The entering pressure may vary between 1 atm and 160 atm and the entering temperature is between 300K and 400K. A total tubular reactor volume of 2m^3 is to be used.

1.3 Overview:

This project is centered around the synthesis of a non-consumable alcohol called methanol. We will be using a packed bed reactor to synthesize this alcohol (methanol) at given conditions considering isobaric, isothermal and pressure drop conditions. Although multiple catalysts can be used to catalyze this process of synthesis, we have been given the responsibility to select the most suitable catalyst for this synthesis. In this project, as you read along, you will see the calculations and equations that were used in the process of reaching our objective

1.4 Meeting Summary:

Date of Meeting	Discussion
4/19/22	General discussions of project
4/23/22	Delegation of tasks to group members
4/30/22	Individual update on progression of project via zoom
5/2/22	Selected group leader to submit project
5/6/22	Final editing and submission

when did you have meeting with instructor?

Reactor System Design and Assumptions:

Figure 1.2 Schematic Diagram

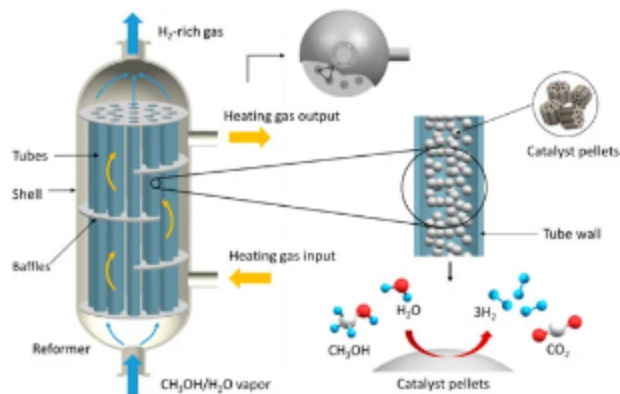


Figure 1.1 Displays a packed bed reactor with multiple tubes designed for methanol synthesis

Reactor dimensions:

Reactor equipment data:

- Catalyst bed void fraction: 40%
- Catalyst density: 1600 kg.m^{-3}
- Tube diameter (i.d.): 3.81 cm
- Overall heat transfer coefficient: $631 \text{ W.m}^{-1} \text{ K}^{-1}$
- Tube diameter (o.d.): 4.20 cm = 0.042m
- Shell side water temperature: 373 K
- Catalyst particle size: 5mm
- Average gas viscosity, assumed constant over all temperature: $7.5 \times 10^{-6} \text{ Pa.s}$
- Number of tubes in the heat exchanger: 250 tubes

Temp range = 300K to 400K

$R = 1.987 \text{ cal.mol}^{-1} \text{ K}^{-1}$

Pressure range = 1atm and 160atm

Reactor volume = 2m³

ASSUMPTIONS:

- STEADY STATE
- NO RADIAL VARIATIONS IN CONCENTRATION, TEMPERATURE, OR REACTION RATE
- REACTION TAKES PLACE ON CATALYST SURFACE

Additional problem information:

Thermodynamic and rate data T is in Kelvin, but R = 1.987 cal.mol⁻¹.K⁻¹. The subscript 1 refers to the methanol reaction, while subscript 2 refers to the water-gas shift reaction. V = 40 dm³

$$K_1 = 131667(0.001987T)^2 \exp \exp \left[\frac{30620}{R} \left(\frac{1}{T} - \frac{1}{298} \right) \right] \left[\frac{\text{dm}^3}{\text{mol}} \right]^2$$

$$K_2 = 103943 \exp \exp \left[\frac{9834}{R} \left(\frac{1}{T} - \frac{1}{298} \right) \right]$$

$$k_1 = 0.933 \times 10^{-6} \exp \exp \left[2.5 \left(\frac{31400}{R} \left(\frac{1}{330} - \frac{1}{T} \right) \right) \right] \left[\left(\frac{\text{dm}^3}{\text{mol}} \right)^2 \text{s}^{-1} \right]$$

$$k_2 = 0.636 \times 10^{-6} \exp \exp \left[\frac{18000}{R} \left(\frac{1}{300} - \frac{1}{T} \right) \right] \left[\frac{\text{dm}^3}{\text{mol.s}} \right]$$

Chemical Reaction Engineering

Using $F_{A0} = F_A \times F_{T0}$ to calculate for A, B, C and D

$$F_{A0} = F_{C0} = \frac{1}{5} \times 300 \text{ mol/s} = 60 \text{ mol/s}$$

$$F_{B0} = \frac{7}{15} \times 300 \text{ mol/s} = 140 \text{ mol/s}$$

$$F_{D0} = \frac{2}{15} \times 300 \text{ mol/s} = 40 \text{ mol/s}$$

$$\rho = \frac{m_s}{v_s}$$

m_s is calculated below:

Molar weight of A (CO): 28kg/kmol = 0.028kg/mol

Molar weight of B (H₂): 2kg/kmol = 0.002kg/mol

Molar weight of C (CH₃OH): 32kg/kmol = 0.032kg/mol

Molar weight of D (H₂O): 18kg/kmol = 0.018kg/mol

Molar weight of E (CO₂): 44kg/kmol = 0.044kg/mol

$m_{D_o} = 0.018 \times 40 = 0.72\text{kg/s}$ for H₂O

$m_{A_o} = 0.028 \times 60 = 1.68\text{kg/s}$ for CO

$m_{B_o} = 0.002 \times 140 = 0.28\text{kg/s}$ for H₂

$m_{E_o} = 0.044 \times 60 = 2.64\text{kg/s}$ for CO₂

Total initial mass flow rate = (1.68+0.28+2.64) kg/s = 4.6kg/s

$$C_{TO} = \frac{P_o}{RT_o}$$

$$C_{TO} = \frac{40}{8.21 \cdot 10^{-1} \cdot 300} \frac{\text{atm}}{\text{atm} \cdot \frac{\text{m}^3}{\text{mol} \cdot \text{K}}} = 1624.89 \frac{\text{mol}}{\text{m}^3}$$

$$\text{If } F_{TO} = C_{TO} v_o$$

Given: $F_{TO} = 300\text{mol/s}$

$$v_o = \frac{F_{TO}}{C_{TO}} = \frac{300 \frac{\text{mol}}{\text{s}}}{1624.89 \frac{\text{mol}}{\text{m}^3}} = 0.18 \frac{\text{m}^3}{\text{s}} \cong 0.2 \frac{\text{m}^3}{\text{s}}$$

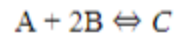
Total initial mass flow rate = (1.68+0.28+2.64) kg/s = 4.6kg/s

Also, density ρ_o can be calculated as follows:

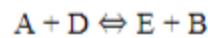
$$\rho_o = \frac{m_o}{v_o} = \frac{4.6 \frac{\text{kg}}{\text{s}}}{0.18 \frac{\text{m}^3}{\text{s}}} = 25.56 \frac{\text{kg}}{\text{m}^3}$$

Given the following equation below we can deduce the mole balance and rate laws as follows

Equation 1: $CO + 2H_2 \rightleftharpoons CH_3OH$



Equation 2: $CO + H_2O \rightleftharpoons CO_2 + H_2$



Mole Balance:

$$\frac{dF_A}{dW} = r_A$$

$$\frac{dF_B}{dW} = r_B$$

$$\frac{dF_c}{dW} = r_c$$

$$\frac{dF_D}{dW} = r_D$$

$$\frac{dF_E}{dW} = r_E$$

Rate laws:

The rate laws are as follows:

$$r_{A1} = -K_1 C_A C_B^2$$

$$r_{A2} = -K_2 C_A C_D$$

Net rate:

$$r_A = r_{A\text{net}} = r_{A1} + r_{A2}$$

$$r_B = r_{B\text{net}} = -K_1 C_A C_B^2 + K_2 C_A C_D$$

$$r_D = K_2 C_A C_D$$

Relative rates:

For equation 1:

$$-r_{A1} = \frac{r_c}{-1} = r_c$$

For equation 2:

$$-r_{A2} = -r_D = r_E = r_B$$

Stoichiometry:

$$C_A = C_{T0} \left(\frac{F_A}{F_T} \right) \cdot \frac{p}{p_0}$$

$$C_B = C_{T0} \left(\frac{F_B}{F_T} \right) \cdot \frac{p}{p_0}$$

$$C_C = C_{T0} \left(\frac{F_C}{F_T} \right) \cdot \frac{p}{p_0}$$

$$C_D = C_{T0} \left(\frac{F_D}{F_T} \right) \cdot \frac{p}{p_0}$$

$$C_E = C_{T0} \left(\frac{F_E}{F_T} \right) \cdot \frac{p}{p_0}$$

Where: $p = \frac{p}{p_0}$ represents pressure drop.

$$\text{Also, } F_T = F_A + F_B + F_C + F_D + F_E$$

Combine:

$$\text{For A (CO):} \quad -k_1(C_A C_B^2 - \frac{C_E}{K_{1eq}}) - k_2(C_A C_D - \frac{C_E C_B^2}{K_{2eq}})$$

$$\text{For B (H}_2\text{):} \quad -k_1(C_A C_B^2 - \frac{C_E}{K_{1eq}}) + k_2(C_A C_D - \frac{C_E C_B^2}{K_{2eq}})$$

$$\text{For C (CH}_3\text{OH):} \quad k_1(C_A C_B^2 - \frac{C_E}{K_{1eq}})$$

$$\text{For D (H}_2\text{O):} \quad -k_2(C_A C_D - \frac{C_E C_B^2}{K_{2eq}})$$

$$\text{For E (CO}_2\text{):} \quad k_2(C_A C_D - \frac{C_E C_B^2}{K_{2eq}})$$

Reactor equipment data:

- Catalyst bed void fraction: 40% • Catalyst density: 1600 kg.m⁻³
- Tube diameter (i.d.): 3.81cm • Overall heat transfer coefficient: 631 W.m⁻¹ .K⁻¹
- Tube diameter (o.d.): 4.20 cm = 0.042m • Shell side water temperature: 373 K
- Catalyst particle size: 5mm • Average gas viscosity, assumed constant over all temperature: 7.5 × 10⁻⁶ Pa.s • Number of tubes in the heat exchanger: 250 tubes

The reactor equipment data are as shown above. We will use 250 tubes and 2m³ for this project

So N_t = 250 tubes, Volume = 2m³

Cross sectional area can be calculated using

$$A = \frac{\pi d^2}{4} N_t$$

$$A = \frac{3.142 \cdot 0.0381^2 \cdot 250}{4} = 0.29 \text{ m}^2$$

$$\text{length, } z = \frac{V}{A} = \frac{2 \text{ m}^3}{0.29 \text{ m}^2} = 7.02 \text{ m}$$

Weight of catalyst, W

$$W = A \rho (1-\phi) z$$

$$W = 0.29 \times 1600 (1-0.4) \times 7.02 = 1920 \text{ kg}$$

Mass velocity, G

$$G = Q\mu = \frac{m}{A}$$

$$G = \frac{4.6}{0.29}$$

$$G = 15.86 \text{ kg/m}^2 \text{ s}$$

$$\begin{aligned} \beta_o &= \frac{G(1-\phi)}{g_s \rho_s D_p \phi^3} \left[\frac{150(1-\phi)\mu}{D_p} + 1.75G \right] \\ &= \frac{15.86(1-0.4)}{1.75 \cdot 56 \cdot 0.0381 \cdot 0.4^3} \left[\frac{150(1-0.4)7.5 \cdot 10^{-4}}{0.0381} + 1.75(15.86) \right] \\ &\quad \beta_o \\ &= 4240.4 \frac{\text{Pa}}{m} \end{aligned}$$

2.3 Modeling Using Polymath (Inputs)

```

differential equations: 6 Auxiliary Equations: 43 Ready for solution
# CHEG 3306 Final Project
# Objective 1
# Group 1
# Janoria Perry
# Oluwatumininu Alade
# Erron Williams
# Dr. Nabila Shamim

# Conditions
T = 330 # 1st simulation Initial Temperature entering reactor [K]
P = 40 # 1st Simulation Initial Pressure entering reactor [atm]
Fto = 300 # Total initial molar flow rate [mol/s]
R = 1.987 # Gas constant [cal/mol*K]
Po = 40 # Assuming isobaric
To = 330 # Assuming isothermal

# Reactor Equipment Data:
cbv = 0.40 # Catalyst bed void fraction
pc = 1600 # Catalyst density [kg/m^3]
di = 0.0381 # Tube inner diameter [m]
do = 0.042 # Tube out diameter [m]
U = 631 # Overall heat transfer coefficient [W m^-1 K^-1]
Dp = 0.005 # Catalyst particle size [m]
Vsc = 7.6 * 10^-6 # Average gas viscosity [Pa.s]
Nth = 250 # Number of tubes in heat exchanger

# Constants
K1 = (131667 * ((0.001987 * T)^2)) * exp((30620 / R) * ((1 / T) - (1 / 298))) # [dm6/s*mol^2]
K2 = (103943) * exp((9834 / R) * ((1 / T) - (1 / 298))) # [dm3/mol]
k1 = (0.933 * 10^-6) * exp(2.5 * ((31400 / R) * ((1 / 330) - (1 / T)))) # [dm6/s*mol^2]
k2 = (0.636 * 10^-6) * exp((18000 / R) * ((1 / 300) - (1 / T))) # [dm3/mol]

# Mole Balance Values
Fco2(0) = 60
W(0) = 0
W(f) = 1920
Fh2(0) = 140
Fco(0) = 60
Fch3oh(0) = 0
Fh2o(0) = 40

# Mole balances
d(Fh2)/d(W) = rh2 # hydrogen
d(Fco)/d(W) = rco # Carbon monoxide
d(Fch3oh)/d(W) = rch3oh # Methanol
d(Fh2o)/d(W) = rh2o # Water
d(Fco2)/d(W) = rco2 # Carbon Dioxide

# Auxiliary Calculations
mo = 4.6 # Total initial mass flow rate [kg/s]
Ac = Nth * 3.14 * (di^2 / 4) # Cross sectional area of reactor
Cto = Po / ((8.2057 * 10^-5) * To) # Initial concentration [mol/m^3]
vo = Fto / Cto # Initial volumetric flow rate [m^3/s]

```

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Fig1.2. Algorithm as abstracted from polymath

Algorithm for pressure drop

```

Differential Equations: 6 | Auxiliary Equations: 43 | Ready for solution

# CHEG 3306 Final Project
# Objective 2
# Group 1
# Janeria Perry
# Oluwatumininu Alade
# Erron Williams
# Dr. Nabila Shamim

# Conditions
T = 380 # 2nd simulation Initial Temperature entering reactor [K]
P = 1 # 2nd Simulation Initial Pressure entering reactor [atm]
Fto = 300 # Total initial molar flow rate [mol/s]
R = 1.987 # Gas constant [cal/mol*K]
Po = 1 # Assuming Isobaric
To = 380 # Assuming Isothermal

# Reactor Equipment Data:
cbvf = 0.40 # Catalyst bed void fraction
pc = 1600 # Catalyst density [kg/m^3]
di = 0.0381 # Tube inner diameter [m]
do = 0.042 # Tube out diameter [m]
U = 631 # Overall heat transfer coefficient [W m^-1 K^-1]
Dp = 0.005 # Catalyst particle size [m]
Vsc = 7.5 * 10^-6 # Average gas viscosity [Pa.s]
Nth = 250 # Number of tubes in heat exchanger

# Constants
K1 = (131667 * ((0.001987 * T) ^ 2)) * exp((30620 / R) * ((1 / T) - (1 / 298))) # [dm6/s*mol^2]
K2 = (103943) * exp((9834 / R) * ((1 / T) - (1 / 298))) # [dm3/mol]
k1 = (0.933 * 10^-6) * exp(2.5 * ((31400 / R) * (1 / 330) - (1 / T))) # [dm6/s*mol^2]
k2 = (0.636 * 10^-6) * exp((18000 / R) * ((1 / 300) - (1 / T))) # [dm3/mol]

# Mole Balance Values
Fco2(0) = 60
W(0) = 0
W(f) = 1920
Fh2(0) = 140
Fco(0) = 60
Fch3oh(0) = 0
Fh2o(0) = 40

# Mole balances
d(Fh2)/d(W) = rh2 # hydrogen
d(Fco)/d(W) = rco # Carbon monoxide
d(Fch3oh)/d(W) = rch3oh # Methanol
d(Fh2o)/d(W) = rh2o # Water
d(Fco2)/d(W) = rco2 # Carbon Dioxide

# Auxiliary Calculations
mo = 4.6 # Total initial mass flow rate [kg/s]
Ac = Nth * 3.14 * (di ^ 2 / 4) # Cross sectional area of reactor
Cto = Po / ((8.2057 * 10^-5) * To) # Initial concentration [mol/m^3]
vo = Fto / Cto # Initial volumetric flow rate [m^3/s]

```

Fig1.3. Algorithm for pressure drop

Results did not show polymath graphs -4

3.1 Data tables

Inlet temperature (K)	330K
Outlet temperature (K)	360K
Inlet pressure (Pa)	40

Outlet Pressure (Pa)	60
Maximum tube-side temperature (K)	375
Location from inlet of maximum temperature(m)	19
Methanol production rate(kgs ⁻¹)	0.629
Reactor length (m)	7.02
Total inlet concentration C _{To} at 330K	1624.89
Rate constant, k ₁ at 330K	9.33x10 ⁻⁷
Equilibrium constant K _c , 1 at 330K	375.95
Rate constant k ₂ at 330K	9.9x10 ⁻⁶
Equilibrium constant K _c , 2 at 330K	20770
Heat of reaction 2 at 330K	-48.98
Heat of reaction 2 at 330K	-19.51

Table for results

Reactor in and out

Flows(mol.s ⁻¹)	196.58
Pressure (Pa)	40
Temperature (K)	330
F _{co}	0.039
F _{H2}	0.189
F _{co2}	0.308
F _{H2O}	0.2

Table for reactor in and out

4. Task 1/ Discussion:

The requirements of this project entails the process necessary to determine the overall process, economical uses, reactor types, and configurations necessary for the optimal conversion

of carbon dioxide necessary for methanol synthesis. The general requirement is to consider a packed bed reactor that will operate isothermally with constant pressure. The initial requirements of the reactor operated with a temperature and pressure of required of 330C and 40atm. The first polymath code in this report represents the values that correspond to the reactor without pressure drop. There were several attempts made to run the polymath algorithm using the differential equation software.

Task three of the report required that the reactor operates with the effects of pressure drop. The second polymath program ran with these paraments and several values were altered after the pressure drop was considered. The program did not run until the correct correlation of final pressure and initial pressure was defined within the program. In order to run the polymath software, the term representing the ratio of partial pressure to initial pressure was rearranged with respect to the final pressure. The code was then able to correctly represent the effects of pressure drop within the packed bed reactor.

Catalyst Selection:

Figure 3.1

Table 2. Effect of Zr on the activity and selectivity for methanol synthesis on Cu-Zn-Al-Zr catalysts (523 K and 5 MPa) [76].

Sample	Atomic Ratio ^a Cu ²⁺ :Zn ²⁺ :Al ³⁺ :Zr ⁴⁺	CO ₂ Conversion (%)	CH ₃ OH Yield (μmol mL ⁻¹ h ⁻¹)	Selectivity (C mol%)	
				CH ₃ OH	CO
Cal.HfTs-0	2:1:1:0	20.2	3433	42.3	57.7
Cal.HfTs-1	2:1:0.9:0.1	21.9	4057	45.8	54.2
Cal.HfTs-3	2:1:0.7:0.3	22.5	4369	47.4	52.6
Cal.HfTs-5	2:1:0.5:0.5	19.5	3745	44.0	56.0
Cal.HfTs-7	2:1:0.3:0.7	15.3	2497	37.1	62.9

^a Nominal atomic ratio in the synthesis mixture.

Copper-based catalysts are best equipped for the synthesis of methanol. The typical configuration of the catalysts that are used for this reaction contains copper, zinc, and aluminum; they are commonly referred to as Cu/ZnO/Al-based catalysts. In the table above the catalyst that has a high amount of aluminum grants the highest selectivity to methanol, while also having a higher CO₂ conversion. The catalyst chosen for the purpose of designing a packed bed reactor capable of synthesizing methanol from carbon monoxide from hydrogen gas is the catalyst Cu/ZnO/Al₂O₃.

The catalyst Cu/ZnO/Al₂O₃ can operate between the temperature parameters of 300K-400K. One of the reactions that take place with methanol synthesis is considered a water-gas shift reaction due to the presence of H₂, and this catalyst is capable of catalyzing at low temperatures.

Since the reactor type is a packed bed; the mole balance algorithm for isothermal and isobaric packed bed reactor with the presence of a catalyst was used to correlate the reaction. were followed in order to correlate variables needed to The algorithm for a packed bed reactor was followed meticulously to determine the feed conditions fo H₂, CO, and H₂O. The

5. Reflection/ Conclusion

This project consisted of the methods necessary to design a packed bed reactor used for methanol synthesis. The materials used to evaluate the necessary design criteria mainly consisted of trial and error using the polymath coding software. The second task within the problem statements required that the reactor operate under isothermal and isobaric conditions. These conditions are much easier to evaluate using the polymath software since most of the assumptions allowed for less calculation.

The polymath coding software created several setbacks due to the immense amount of numerical values and reactor specifications and constraints. The initial calculation was considered by the standard algorithms used for a packed bed reactor. However, after the algorithm was used there were different unit conversions, process modifications, and additional tasks necessary to complete all of the essential calculations necessary to complete the final code. Once the polymath code was able to run there were so many different variables that appeared to be too small or too large given the data set. The results mentioned in the discussion portion of the report contain graphical data that was created using the polymath software, and each graph represents the molecular flow rates and concentration across the weight of the catalyst.

References

"Energies | Free Full-Text | Modeling and Design of a Multi-Tubular Packed-Bed Reactor for Methanol Steam Reforming over a Cu/ZnO/Al₂O₃ Catalyst." *MDPI*, Multidisciplinary Digital Publishing Institute, <https://www.mdpi.com/1996-1073/13/3/610>. Accessed 6 May 2022.

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BELOW AVERAGE

Below Average Student Original Graded Assignment

Prairie View A&M
Roy G. Perry College of Engineering



Chemical Reaction Engineering
CHEG 3306 Final Project

Submitted by: Shelton A., Berenice R.
To: Dr. Nabila Shamim
Due Date: May 6, 2022

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list of tables and figures -2

Executive Summary

In this project, our team was required to design a shell and tube packed bed reactor for methanol synthesis. We used Polymath rather than MATLAB to do this assignment due to the simplicity of the software along with the group's comfortability level. To complete this project multiple tasks must be done. First, we must discuss the economic side of things as it relates to our overall process along with the different conditions of the process and the characteristics of our catalyst. The next thing that had to be done was to determine the entering conditions of the temperature and pressure that would optimize the production of methanol for our system.

The next thing we had to accomplish was to go through with the design process of our shell and tube reactor while following the optimal feed conditions set in place. During this part the temperature in the shell can be changed by adjusting the steam pressure to different values. In our design the things included are the reactor dimensions/number of tubes, the reactor conditions along with its composition pressure and temperature profile, and a mechanical sketch of the reactor. While accomplishing this part of our tasks, we also must determine the effect of the change in our ratio of feed for H_2 to CO , ratio of feed for H_2O to CO , and our assumed heat transfer coefficient, U .

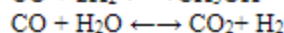
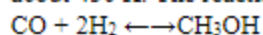
Introduction

1.1 Objective

- To demonstrate your understanding of designing a packed bed reactor.
- Show that you can calculate the required design taking heat, pressure drop and changing physical properties into account.
- Design and create a plan of action that you will follow to achieve your goal.
- To reflect afterwards on your group's progress and judge how you followed your plan.

1.2 Problem Statement

A new catalyst has been proposed for the synthesis of methanol from carbon monoxide and hydrogen gas. This catalyst is reasonably active between temperatures of 330 K to about 430 K. The reactions to be considered are:



The reactions are elementary and occur in a reactor containing tubes packed with a precious metal catalyst on a silica support. Heat is removed from the reactor by generating steam on the shell side of the tubes. The feed consists of 7/15 hydrogen gas, 1/5 carbon monoxide, 1/5 carbon dioxide, and 2/15 steam. The total flow rate is 300 mol.s⁻¹. The entering pressure may be varied between 1 atm and 160 atm and the entering temperature between 300K and 400 K. A total tubular reactor volume of 2 m³ is to be used.

1.3 Overview

This project, our team will identify, develop, design, and calculate the missing values provided in the problem statement. Next, we will choose the best suited catalyst for methanol process reaction. Then, we will calculate using polymath as our program to find out the desired product of the reaction. Finally, from gathering literature resources and calculating the objectives, we will be able to create and utilize a packed bed reactor to find the outcome for methanol synthesis process.

1.4 Update Meeting Summary

April 18- Discussed the layout of the project

April 23- literature research and begin polymath

May4-Begin editing the letter report

May 6- Finish the letter report and find results for polymath

Methods

2.1 Reaction System Design and Assumptions

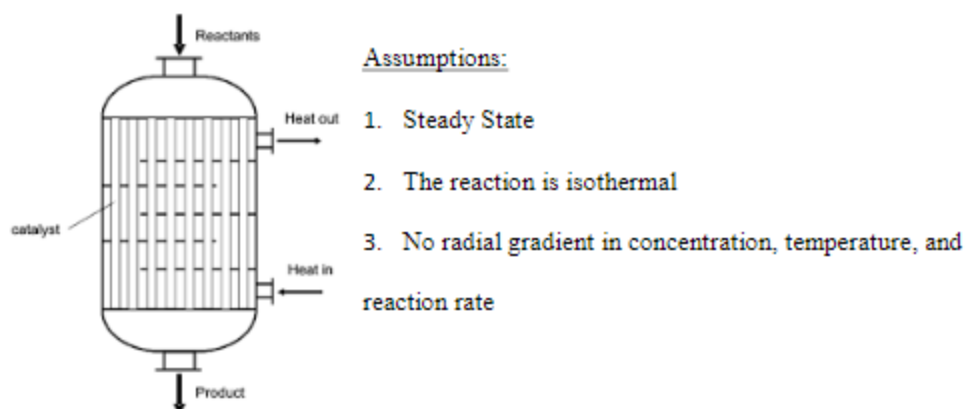


Figure 1: Packed Bed Reactor

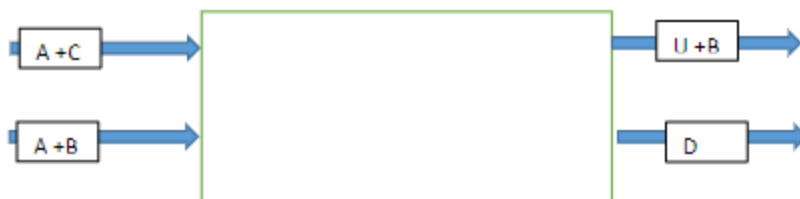


Figure 2: PBR Gas-Phase Diagram

In Figure 1: Packed Bed Reactor design, depicts the methanol process we will be using to find in and out flows of our reaction. This image shows the catalytic membrane flowing in to out to acquire the final desired product; By assuming we have 250 tubes in the heat exchanger, the reaction will be under isobaric and isothermal conditions. From Figure 2, a schematic gas phase diagram of packed bed reactor indicates the process calculations of the methanol process.

2.2 Chemical Reaction Engineering

Mole Balance

$$\frac{dFA}{dW} = r_A'$$

$$\frac{dFB}{dW} = r_B'$$

$$\frac{dFC}{dW} = r_C'$$

Rate Law

$$\diamond \quad r_{1A} = K_{1A} C_A C_B^2$$

$$> \quad r_{-1A} = -K_{1A} C_D$$

$$> \quad r_{1A} = K_{1A} (C_A C_B - \frac{C_D}{K_c})$$

$$\diamond \quad r_{2A} = K_{2A} C_A C_B$$

$$> \quad r_{-2A} = -K_{2A} C_B C_U$$

$$> \quad -r_{2A} = K_{2A} (C_A C_B - \frac{C_B C_U}{K_c})$$

Stoichiometry

$$C_A = C_{T0} \frac{F_A}{F_T} P$$

$$C_B = C_{T0} \frac{F_B}{F_T} P$$

$$C_C = C_{T0} \frac{F_C}{F_T} P$$

$$\frac{dp}{dW} = -\frac{\alpha}{2p} (1 - \epsilon X)$$

$$\epsilon = y_{A0} \delta$$

$$FA = FA0(1 - X)$$

$$FB = FBO(1 - X)$$

$$FC = FCO(1 - X)$$

$$FD = FDO(1 - X)$$

$$FU = FUU(1 - X)$$

$$CD = CTO \frac{FD}{FT} P$$

$$CU = CTO \frac{FU}{FT} P$$

$$FT = FA + FB + FC + FD$$

to calculate pressure drop calculate alpha and beta -5

Molar Flow Rates

$$H_2F_A = \frac{7}{15} * 300 \frac{\text{mol}}{\text{s}} = 140 \frac{\text{mol}}{\text{s}}$$

$$CO_2F_U = \frac{1}{15} * 300 \frac{\text{mol}}{\text{s}} = 60 \frac{\text{mol}}{\text{s}}$$

$$COF_B = \frac{1}{5} * 300 \frac{\text{mol}}{\text{s}} = 60 \frac{\text{mol}}{\text{s}}$$

$$H_2OF_C = \frac{2}{5} * 300 \frac{\text{mol}}{\text{s}} = 40 \frac{\text{mol}}{\text{s}}$$

2.3 Modeling using Polymath

```

d(FH2)/d(W) = FH2 # molar flow rate of H2
FH2(0) = 7
d(FCO2)/d(W) = rCO2 # molar flow rate of CO2
FCO2(0) = 3
d(FCH3OH)/d(W) = rCH3OH # molar flow rate of CH3OH
FCH3OH(0) = 0
d(FH2O)/d(W) = rH2O # molar flow rate of H2O
FH2O(0) = 2
d(FCO2H)/d(W) = rCO2H # molar flow rate of CO2H
FCO2H(0) = 3

FT = FCO2 + FH2 + FCH3OH + FH2O + FCO2H
r1 = k1 * (CO2 * CH2 - 2 * CH3OH / K1)
r2 = k2 * (CO2 * CH2 - 2 * CO2H * CH2 / K2)
# number is found using the temperature in Part 2
k1 = 0.333 * 10^-6 * exp(2.6 * (31400 / 1.987 * (1/330 - 1/T)))
k2 = 0.636 * 10^-6 * exp(18000 / 1.987 * (1/300 - 1/T))
K1 = 121667 * (0.01987 * T)^2 * exp(36326 / 1.987 * (1/T - 1/298))
K2 = 163943 * exp(9834 / 1.987 * (1/T - 1/298))
T = 360 # optimal temperature

rCO2 = -r1 - r2
rH2 = -2 * r1 + r2
rH2O = 0
rCH3OH = r1
rCO2H = r2
rCO2H = r2

CO2 = CTo * (FCO2 / FT) * p
CH2 = CTo * (FH2 / FT) * p
CH3OH = CTo * (FCH3OH / FT) * p
H2O = CTo * (FH2O / FT) * p
CO2H = CTo * (FCO2H / FT) * p

d(p)/d(W) = -alpha / (2 * p) * (FT / FT0)
p(0) = 10 # optimal pressure
V = 2 # reactor volume
CTo = FT0 / V
alpha = 0.002 # check for correct alpha

```

Figure 3: Polymath algorithm

```

d(p)/d(W) = -alpha / (2 * p) * (FT / FT0)
p(0) = 10 # optimal pressure
FT0 = 15 # initial flowrate
V = 2 # reactor volume
CTo = FT0 / V
alpha = 0.002 # check for correct alpha

```

Results

1.1 Data Tables

Calculated values of DEQ variables

Variable	Initial value	Minimal value	Maximal value	Final value
1 W	0	0	200.	200.
2 FH2	7.	1.655121	7.	1.202181
3 FCO	3.	0.003203	3.	0.003203
4 FCH3OH	0	0	2.900214	2.931179
5 FH2O	3.	1.834462	3.	1.404462
6 FCO2	3.	2.	3.065538	3.065538
7 p	10.	9.987879	10.	9.987879
8 pT	15.	9.639479	15.	9.127643
9 FT0	15.	15.	15.	15.
10 V	2.	2.	2.	2.
11 T	360.	360.	360.	360.
12 k1	0.0200726	0.0200726	0.0200726	0.0200726
13 k2	9.753E-05	9.753E-05	9.753E-05	9.753E-05
14 K1	9.134248	9.134248	9.134248	9.134248
15 K2	5951.149	5951.149	5951.149	5951.149
16 CT0	7.5	7.5	7.5	7.5
17 CCH3OH	0	0	24.29645	24.82932
18 CCO2	15.	15.	35.13084	35.13084
19 CH2	35.	8.752894	35.	9.863504
20 CCO	15.	0.0269134	15.	0.0269134
21 r1	368.8348	-0.0002513	368.8348	-0.0002474
22 r2	1.792098	0.0002513	1.792098	0.0002513
23 rCO	-370.8269	-370.8269	-3.953E-06	-3.953E-06
24 rH2	-735.8775	-735.8775	0.0007657	0.000746
25 rH2O	1.792098	1.792098	-0.0002513	-0.0002513
26 rCH3OH	368.8348	-0.0002513	368.8348	-0.0002474
27 CH2O	10.	10.	16.46408	15.85843
28 rCO2	1.792098	0.0002513	1.792098	0.0002513
29 alpha	0.002	0.002	0.002	0.002

Table 1: Tabular Information

1.2 Results

Differential equations

- $d(FH2)/d(W) = rH2$
molar flow rate of H2
- $d(FCO)/d(W) = rCO$
molar flow rate of CO
- $d(FCH3OH)/d(W) = rCH3OH$
molar flow rate of CH3OH
- $d(FH2O)/d(W) = rH2O$
molar flow rate of H2O
- $d(FCO2)/d(W) = rCO2$
molar flow rate of CO2
- $d(p)/d(W) = -\alpha / (2 - p) = (FT / FT0)$

Explicit equations

- $FT = FCO + FH2 + FCH3OH + FH2O + FCO2$
- $FT0 = 15$
initial flowrate
- $V = 2$
reactor volume
- $T = 360$
optimal temperature
- $k1 = 0.933 \cdot 10^{-6} = \exp(2.5 \cdot (31400 / 1.987 \cdot (1 / 330 - 1 / T)))$
- $k2 = 0.626 \cdot 10^{-6} = \exp(18000 / 1.987 \cdot (1 / 300 - 1 / T))$
- $K1 = 131667 \cdot (0.001987 \cdot T)^{-2} = \exp(30620 / 1.987 \cdot (1 / T - 1 / 298))$
- $K2 = 103943 \cdot \exp(9834 / 1.987 \cdot (1 / T - 1 / 298))$
- $CT0 = FT0 / V$
- $CCH3OH = CT0 \cdot (FCH3OH / FT) = p$
- $CCO2 = CT0 \cdot (FCO2 / FT) = p$
- $CH2 = CT0 \cdot (FH2 / FT) = p$
- $CCO = CT0 \cdot (FCO / FT) = p$
- $r1 = k1 \cdot (CCO \cdot CH2^2 - CCH3OH / K1)$
- $r2 = k2 \cdot (CCO \cdot CH2^2 - CCO2 \cdot CH2 / K2)$

the format is not clear -2

Figure 5: Variable Information

```

15 r2 = k2 * (CCO * CH2 ^ 2 - CC02 * CH2 / K2)
16 rCO = -r1 - r2
17 rH2 = -2 * r1 + r2
18 rH2O = -r2
19 rCH3OH = r1
20 CH2O = CTo * (FH2O / FT) * p
21 rCO2 = r2
22 alpha = 0.002

```

check for correct alpha

check polymath coding, the increase was very sharp. it is not optimized condition -3

Figure 6: Variable Information continued

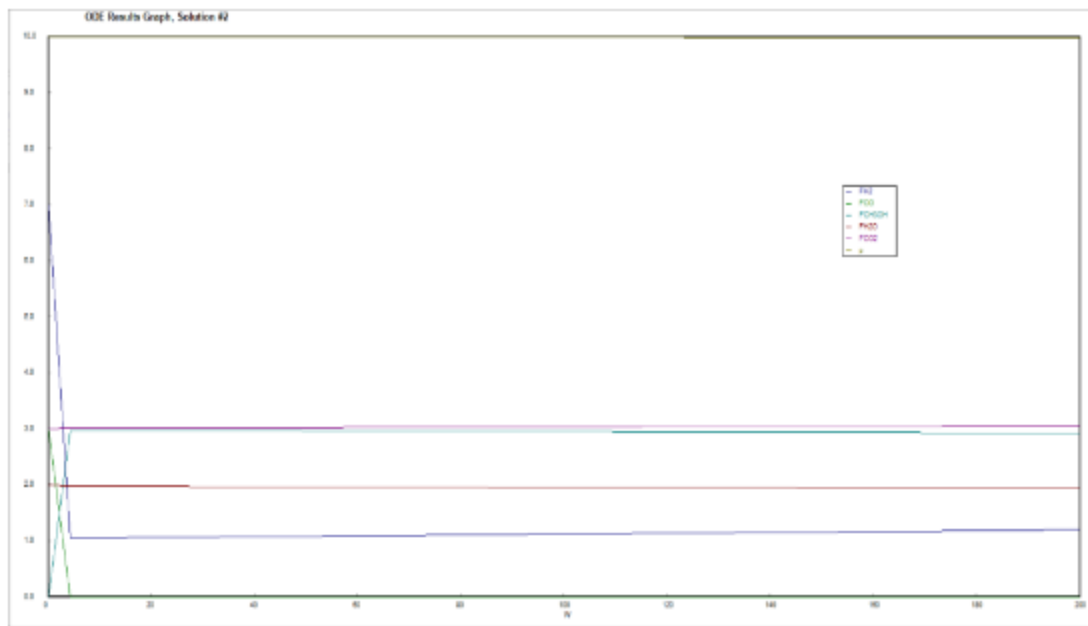


Figure 7: Polymath Graph

Figures 3-7 and Table 1 shown above both show the algorithms, problem statement and the variables found.

what does the graph tells you -2 not polymath graph

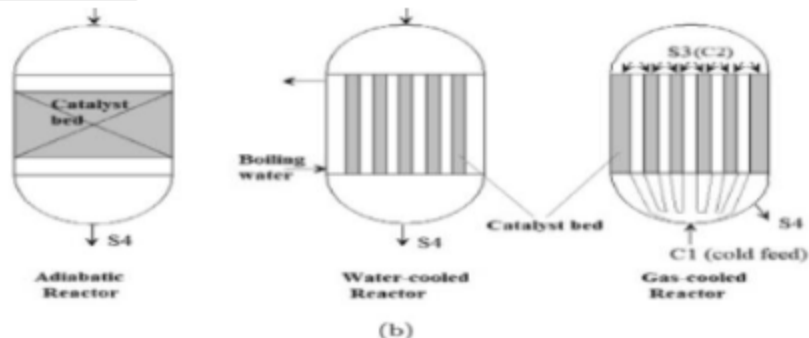
Overall Process

The process of methanol synthesis offers many challenging opportunities for sustainable development. For starters, methanol can be used as a basis to produce many different chemicals such as acetic acid, methyl tertbutyl, and dimethyl terephthalate, etc. In the overall process methanol is produced by mixing CO, CO₂, and H₂ while using copper and zinc-based catalyst. These catalysts are usually active around 200 degrees Celsius.

Economics

The market for Methanol (MeOH) will be increasing in the next few years. Syngas, which is gray MeOH, is usually used to produce methanol. When performing Methanol synthesis engineers have to take production costs into account. The production costs include both the operating costs and the material costs. The capital costs are comprised of the cost of the MeOH synthesis reactor, compressor, distillation, and the supplementary cost. The operating costs consist of the raw material costs, electricity, labor, maintenance. Etc. All these different costs must be considered when choosing the right kind of reactor and chemicals for use.

Process Conditions



In most processes involving methanol synthesis the methanol is produced at pressures ranging from 50-100 bar and 250°C-300°C. In our process our T_0 started at 330 and our P_0 started at 40 atm. During the process we tried to raise the temp to 380°C and lower the pressure to 1 atm.

Reactor Types and Configurations

In this project our team decided to use a water-cooled reactor as it showed advantages in efficient heat removal, low hot-spot, temperature, and a relatively wide range of inlet temperature for control.

Type of Catalyst

The greenhouse effect of carbon dioxide has been recognized to be one of the most serious problems on earth and several countermeasures have been proposed so far. The idea of choosing a catalyst for the synthesis of methanol from carbon monoxide and hydrogen gas is essential. From gathering data and reading journals, our group decided to pick Cu/ZnO-based catalysts. Cu/ZnO- based catalyst research from "Development of copper/zinc oxide-based multicomponent catalysts for methanol synthesis from carbon dioxide and hydrogen" suggest that the multicomponent catalyst developed in the present work is very stable for a long period in continuous methanol synthesis operation therefore it is best suited for this project as the catalyst.

Typical Conversion and End product usage

Methanol is made using high selectivity, however there are a few amounts of side products formed. The methanol synthesis typically conducts around 200 C and around 4 MPa. The maximum theoretical conversion is between 60% to 70% conversion.

Reflection/Conclusion

Our team had encountered obstacles such as deadlines for other assignments. Sticking to the plan accurately was not achievable, however we were able to accommodate by comparing our schedules and trying to make up the days that we missed to meet. This included meeting on the weekends and working early in the mornings to compensate for the missing days. If there was a way to restart this project, our team would outline the priorities and have this project marked as our top priority. In this project, we learned how to manage our time wisely, work as a group and team, and manage priorities at the last minute. We also learned the importance of creating deadlines to improve our work efficiency. In conclusion

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