AIChE

The Global Home of Chemical Engineers

2020 - 2021
Student Design Competition
Problem Statement & Rules

If there are any questions about the design problem, Student Chapter Advisors and Design Assignment Instructors are directed to contact studentchapters@aiche.org.

Please read the rules before preparing and submitting the solution to AIChE.

AIChE 2020 - 2021 Student Design Competition

Dear Chemical Engineering Department Heads and Student Chapter Advisors,

We are pleased to send you the 2020 - 2021 AIChE Student Design Competition statement. Please forward this problem statement to those faculty teaching design courses.

In order to maintain the integrity of this competition, all Chemical Engineering Departments are asked to familiarize themselves with these rules before assigning this problem to students. **Chemical Engineering Departments, including advisors, faculty, or any other instructors, cannot provide technical aid specifically directed at the solution of the AIChE Student Design Competition if students plan on submitting to the contest. Please inform your Chemical Engineering Department about the rules for this competition so that they do not provide technical aid that would be a violation of the competition rules.**

It is the responsibility of the Design Professor to choose the best solution or solutions, not to exceed two from each category (individual and team), from his or her University and submit them to AIChE for consideration in the contest. The Design Professor will be asked to upload the winning solution(s) using an online form. Design Professors should use the 2021 AIChE Design Competition Entry Form to collect the information needed from each student (including name, AIChE Member ID, contact information and dates of problem assignment/completion).

Please remember that active AIChE Student Membership is required in order for solutions to be considered. All student members must login and renew their membership every year to keep it active. Students can join or renew online at http://www.aiche.org/students/. Any non-member submissions will not be considered.

All solutions must be submitted no later than **11:59 pm US Eastern Time** on **Friday, June 11, 2021.**

- Team Submissions: https://chenected.wufoo.com/forms/2021-student-design-competition-team/

- Individual Submissions: https://chenected.wufoo.com/forms/2021-student-design-competition-individual/

If there are any questions, please contact AIChE at studentchapters@aiche.org. Thank you for your support of this important student competition.

Sincerely,
Harpreet Singh
AIChE Student Programs

Scott C. Rowe
University of Colorado Boulder Chemical and Biological Engineering

2020 – 2021 AIChE Student Design Competition Rules

1. The 2020 - 2021 Student Design Competition is designed to be solved either by an individual chemical engineering student working entirely alone, or a group of no more than four students working together. Solutions will be judged in two categories: individual and team.
2. A period of no more than **ninety (90) days** is allowed for completion of the solution. The finished report should be submitted to the faculty advisor within the 90-day period. Students & faculty advisors should include the date assigned & the date completed along with their signature on the competition entry form.
3. It is to be assumed that the statement of the problem contains all the pertinent data except for those available in handbooks and literature references. The use of internet, textbooks, handbooks, journal articles, and lecture notes is permitted.
4. Students may use any available commercial or library computer programs in preparing their solutions. Students are warned, however, that physical property data built into such programs may differ from data given in the problem statement. In such cases, as with data from literature sources, values given in the problem statement are most applicable. Students using commercial or library computer programs or other solution aids should so state in their reports and include proper references and documentation. Judging, however, will be based on the overall suitability of the solutions, not on skills in manipulating computer programs.
5. **Chemical Engineering Departments, including advisors, faculty, or any other instructors, cannot provide technical aid specifically directed at the solution of the AIChE Student Design Competition if students plan on submitting to the contest. For example, if the problem statement asks for students to design a Hydrogen production process, faculty members should not be directly telling the students how to design this process or suggesting to them which process to use.**

   Students are permitted to ask generalized questions to faculty members and outside experts while working on this problem. For example, if students are designing a Hydrogen production process and they have 2 production methods in mind, the students may ask a Faculty Member and/or professional with expertise in Hydrogen production about their experiences working with the different methods so that they can make an informed decision on which method to choose for their design. Students are also permitted to ask for assistance on how to use process simulation software. If there are any questions about the distinction of what aid can be provided to students who are working on this problem for the contest, please contact studentchapters@aiche.org.

6. **All students working on this problem statement are asked to not share or discuss the topic of this problem statement with other students from their University or from other Universities while they are working on the problem. Students should be aware that sharing the problem statement topic with students from other Universities might be giving those other Universities an unfair advantage in this competition, as those Universities may not**

have started their 90 day time limit yet. If there are any questions about this rule, please contact studentchapters@aiche.org.

7. Solutions will be graded on (a) substantial correctness of results and soundness of conclusions, (b) ingenuity and logic employed, (c) accuracy of computations, and (d) form of presentation.
8. Accuracy of computations is intended to mean primarily freedom from mistakes; extreme precision is unnecessary.

2020 - 2021 AIChE Student Design Competition Eligibility

- Please remember that active AIChE Student Membership is required in order for solutions to be considered. All student members must login and renew their membership every year to keep it active. Students can join or renew online at http://www.aiche.org/students/. Any non-member submissions will not be considered.
- Entries must be submitted either by individuals or by teams of no more than four students.
- Each Faculty Advisor should select the best solution or solutions, not to exceed two from each category (individual and team), from his or her University and submit them per the instructions.

2020 - 2021 AIChE Student Design Competition Timeline

- A period of no more than ninety (90) days is allowed for completion of the solution.
- The finished report should be submitted to the faculty advisor within the 90-day period.
- Students & faculty advisors should include the date assigned & the date completed along with their signature on the competition entry form.

2020 - 2021 AIChE Student Design Competition Report Format

The body of the report must be suitable for reproduction, that is, computer-generated and in a printable format. The competition rewards a strong use of graphics, plots, infographics, and tables for information conveyance. This report should include the following components. Write the document as an engineer making a report and recommendation to a client.

Study Estimate
Toppings Refinery Retrofit in Kirkuk, Iraq

1. Letter of Transmittal
2. Cover Page
3. Executive Summary
4. Table of Contents
5. Table of Figures
6. Table of Tables
7. Brief Process Description
8. PFD (label Utilities, Stream Conditions, Flows & Key Components)
    a. Reactor Process Flow Diagram for feed "K"
    b. Extraction Process Flow Diagram for feed "K"
    c. Distillation Process Flow for Diagram for feed "K"
9. Economic Analysis and Sensitivities
10. Process Safety
    a. Inherent Safety Evaluation
    b. Process Safety Management
        i. Process hazards
        ii. P&ID of the Major Fractionator
        iii. Uncongested Vapor Cloud Deflagration
    c. Safety Summary
11. Conclusions
12. Appendix
    a. Reactor Train Detail

        (List modeling assumptions within a brief description of this operation that explains use of a swing reactor and considerations for catalyst deactivation. Delineate the kinetic equations and tabulate all kinetic parameters. Explain the choice of operating temperature(s), isobaric section pressure, and hydrogen recycle ratio. Mention any innovation(s) in reaction execution. Itemize the bare module capital cost of equipment, including catalyst. Show the yearly operating costs, including labor and utilities, for feed "K.")
    b. Exactor Section Detail

(List modeling assumptions within a brief description of this operation. Calculate the financial benefit of sulfolane recycle. Mention any innovation(s) within the extraction section. Itemize the bare module capital cost of equipment and show the temperature profiles of any distillation fractionators for feed "K." Show the yearly operating costs, including labor and utilities, for feed "K.")

c. Distillation Section Detail

(List modeling assumptions within a brief description of this operation that explains separation difficulty with reference to the relative volatilities of Benzene, Toluene, and para-Xylene. Mention any innovation(s) within the distillation section. Itemize the bare module capital cost of equipment and show the temperature profiles of distillation fractionators for feed "K." Show the yearly operating costs, including labor and utilities, for feed "K.")

13. References

- **The solution itself should not reference the students' names or University. Please expunge all such references from the solution. This is so the solutions can be anonymous to the graders when they are choosing the winners.**
- Final submission of solutions to AIChE must be in electronic format (PDF and MS-Word). The full report must be 50 pages or less for all text, appendix and graphics. The final submission to AIChE must consist of no more than 2 electronic files.
- There should not be any variation in form or content between the solution submitted to the Faculty Advisor and that sent to AIChE. The Student Chapter Advisor, or Faculty Advisor, sponsoring the student(s) is asked to maintain the original manuscript(s).

2020 - 2021 AIChE Student Design Competition Submission Instructions

1. Use the accompanying word document titled "2021 AIChE Design Competition Entry Form to collect the information needed from each student (including name, AIChE Member ID, contact information and dates of problem assignment/completion).

2. Upload the solution file(s) and entry form documents online by **11:59 pm US Eastern Time** on **Friday, June 11, 2021.**
   - Team Submissions: https://chenected.wufoo.com/forms/2021-student-design-competition-team/

   - Individual Submissions: https://chenected.wufoo.com/forms/2021-student-design-competition-individual/

2020 - 2021 AIChE Student Design Competition Awards

There are two categories of awards to be given in both the individual and team categories. The first category is for the best overall design. There are additional awards available for the best application of inherent process safety principles in the design.

Below is a complete list of awards available for the 2020 - 2021 AIChE Student Design Competition:

- Team Awards, Best Overall Design
  - 1st Prize (The William Cunningham Award)-$600 *to be divided equally among team members* & Certificate
  - Honorable Mention - Certificate
- Individual Awards, Best Overall Design
  - 1st Prize (The A. McLaren White Award)-$500 & Certificate
  - 2nd Prize (The A.E. Marshall Award)-$300 & Certificate
  - 3rd Prize (The Omega Chi Epsilon Award)-$200 & Certificate
- Safety and Health Division Student Design Competition Award for Safety
  - 4 awards available (from both individual & team submissions)- $600 *to be divided equally among team members* & Certificate
  - Team Design Award (The Jack Wehman Design Award)- $300 *to be divided equally among team members* & Certificate
  - Individual Design Award (The Walter Howard Design Award)- $200 & Certificate

2020 - 2021 AIChE Student Design Competition Problem Statement

Toppings Refinery Retrofit

Business Context

You work at a domestic engineering construction and procurement firm (EPC). Your supervisor just assigned you an opportunity for international expansion in hydrocarbons processing. You assembled your team and demanded coffee, a provisional PFD, and documentation from your summer intern, who provided only the provisional PFD and documentation... Your client, Mr. Abbasi, will assess your proposal with management 90 days from now to evaluate technical and financial feasibility.

Study Estimate

Customer: Mr. Abbasi (COO), (company withheld), Kirkuk Iraq

Despite immense regional oil wealth, Iraqi Kurdistan has historically imported gasoline. The local economy has previously lost $3B annually because indigenous oil was exported at low prices, but expensive refined fuels were imported (Brookings Institute). Numerous wildcat "teapot" and toppings refineries have proliferated to supply this hydrocarbon shortfall. The Iraqi government is now closing these facilities and rehabilitating larger refineries whose product safety, operational standards, and efficiency are superior (rudaw.net).

Mr. Abbasi runs a small toppings refinery (**35,000 barrels per day**) in Kurdistan that processes light sweet Kirkuk crudes that are rich in benzene and low in sulfur. Inevitably, Mr. Abbasi suspects that the government, which is striving towards Western refining standards, might cease his operations if products from his facility continue to harbor hazardous benzene from his feedstocks. He hopes to process naphtha from the local crudes to separate salable benzene without losses in fuels revenue. He seeks a study estimate for a **fixed bed continuous catalytic reformer** that upgrades heavier naphtha into gasoline while providing benzene, Toluene, and Xylenes (BTX) as lucrative byproducts. A desulfurizer, typically used to preprocess reformer feed, is outside the scope of this proposal.

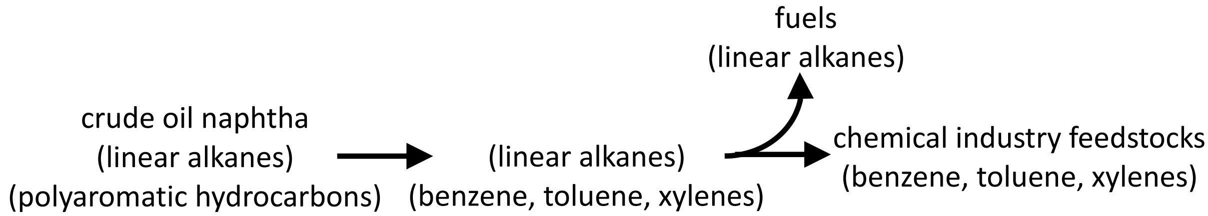
Technical Objectives and Data

Process Description

Oil is a blend of hydrocarbons whose "naphtha" fraction is distilled into gasoline and diesel fuels. Catalytic reforming reacts hazardous cyclic and polyaromatic hydrocarbons within naphtha into benzene, toluene, and xylenes (BTX).[1] This operation removes toxic feedstock constituents from

[1] Kent JA (editor) Riegel's Handbook of Industrial Chem. Springer.
McKetta JJ (editor) Encyclopedia of Chemical Processing & Design. CRC Press.

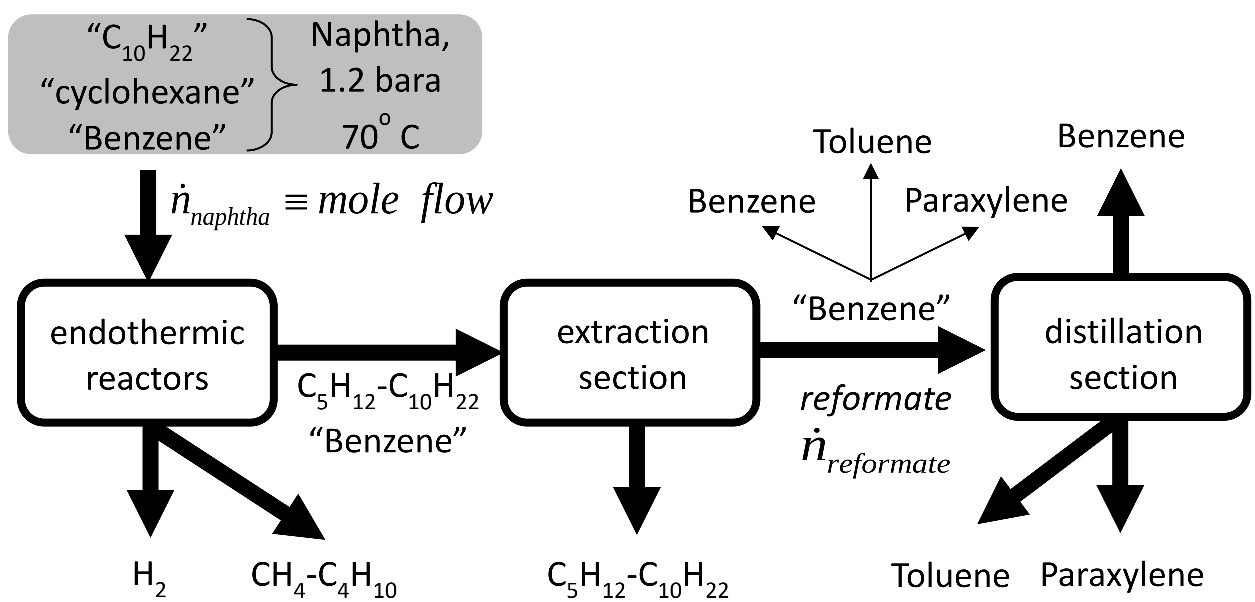
refined fuels, especially benzene and polyaromatic hydrocarbons, as salable aromatics valued by the chemicals industries.



Crude oil in Iraqi Kurdistan has an extremely complex chemical composition. To simplify analysis and cost estimation proxy components can mimic the broad naphtha composition expected in practice. Herein naphtha from expected refinery crude feeds TQ1 or K are represented as follows:[2]

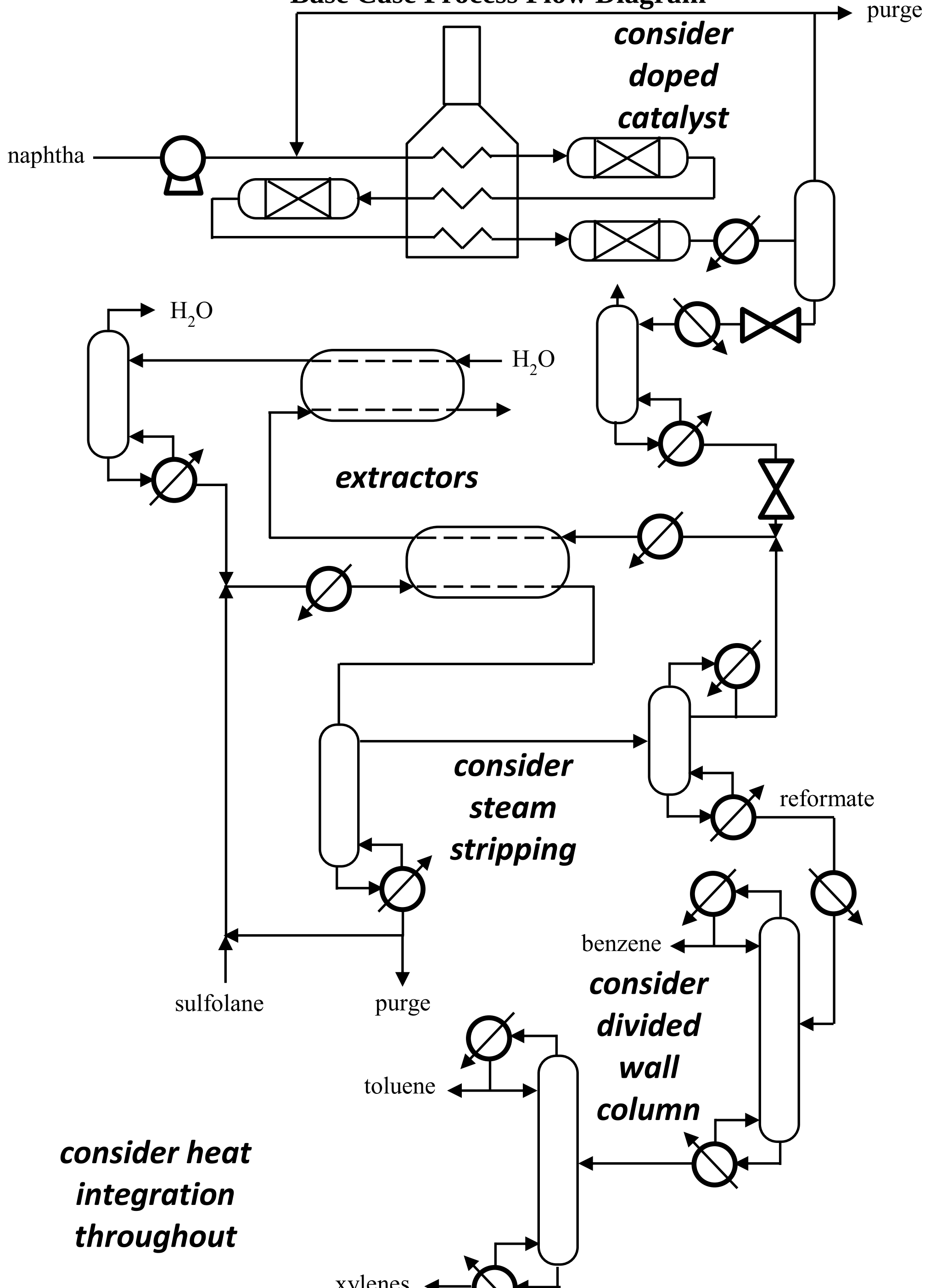
		crude oil	
		TQ1	K
	naphtha % volume of crude	28	20
	specific gravity	0.7308	0.749
naphtha proxy components	n-decane mol%	77.8	59.7
	cyclohexane mol%	20.6	31.3
	benzene mol%	1.6	9

Robust process simulations should converge for either feed, although feed K is of greatest interest. Packed bed reactors convert naphtha cyclohexane, which represents all feed cycloalkanes and polyaromatic hydrocarbons, into benzene, which represents all aromatics. High reactor temperatures also crack feed alkanes, represented by decane, into lighter species. Overall three operations isolate valuable aromatics to produce cleaner fuels:



[2] Karim AR, Khanaqa P & Shukur DA (2017) "Kurdistan crude oils as feedstock for production of aromatics." *Arabian J. of Chem.*, v. 10, pg. S2601-S2607.

Base Case Process Flow Diagram[3]



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[3] Blahusiak M et al. (2018) “Insights into the selection & design of fluid separation processes.” Sep. & Purification Tech., vol. 194, pg. 301-318.

Kluksdahl HE. (1982) “The enhancement of platinum’s catalytic activity by rhenium & other elements.” In Precious Metals. Guindy M.I. (editor) Pergamon Press.

Bishara A, Stranislaus A & Hussain SS (1984) “Effect of feed composition & operating conditions on catalyst deactivation & effect on product yield & quality during naphtha catalytic reforming.” *Applied Catalysis*, vol. 13, pg. 113-125.

Premkumar R & Rangaiah GP (2009) “Retrofitting conventional column systems with dividing-wall columns.” *Chem. Eng. Research & Design*, vol. 87, iss. 1, pg. 47-60.

Once a simulation template is established that harbors the needed physical property packages (see below), draft simulations of the process's three major operations can be built simultaneously by assuming perfect upstream reaction and/or separations. However, before "reformate" entry into the distillation section the components represented by reformate "benzene" must be instantiated.[4] Namely, the mole fractions of chemical components represented by benzene should be calculated:

$$x_{reformate,benzene} = \frac{\dot{n}_{naphtha} x_{naphtha\ benzene} + (\dot{n}_{reformate} - \dot{n}_{naphtha} x_{naphtha\ benzene}) * 0.11}{\dot{n}_{reformate}}$$

$$x_{reformate,toluene} = \frac{(\dot{n}_{reformate} - \dot{n}_{naphtha} x_{naphtha\ benzene}) * 0.55}{\dot{n}_{reformate}}$$

$$x_{reformate,\,para-xylene} = \frac{(\dot{n}_{reformate} - \dot{n}_{naphtha} x_{naphtha\ benzene}) * 0.34}{\dot{n}_{reformate}}$$

Where x refers to mole fraction and $\dot{n}$ refers to mole flow. A base-case process flowsheet, which labels the reformate stream, is shown on the prior page. Although major process operations can be drafted separately, ***ultimately all operations should reside within a single linked simulation.***

Aspen HYSYS and other process simulators generally use reliable property information for hydrocarbons separations. Vapors can be assumed ideal while the NRTL VLE and LLE thermodynamic packages are recommended for liquid modeling in distillation columns and extractors respectively, ***but review binary interaction parameters for abnormalities***. Reaction kinetics for cycloalkane ("cyclohexane" proxy component) dehydrogenation are as follows:[5]

$$C_6H_{12} \rightarrow C_6H_6 + 3H_2$$

$$rate = 9.4928*10^{13} e^{\frac{-160506.4}{8.314T}} P_{C_6H_{12}} - 8.2728*10^{-4} e^{\frac{52170.4}{8.314T}} P_{C_6H_6} P_{H_2}^3$$

$$rate \equiv kmol/(m^3 hr), \qquad P \equiv MPa, \qquad T \equiv Kelvin$$

Reaction kinetics for cycloalkane ("cyclohexane" proxy component) cracking are as follows:[5]

$$C_6H_{12} + 2H_2 \rightarrow 0.4C_5H_{12} + 0.4C_4H_{10} + 0.4C_3H_8 + 0.4C_2H_6 + 0.4CH_4$$

$$rate = 3.6704*10^{21} e^{\frac{-287756.8}{8.314T}} P_{C_6H_{12}}$$

$$rate \equiv kmol/(m^3 hr), \qquad P \equiv MPa, \qquad T \equiv Kelvin$$

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[4] adapted from Wittcoff, H.A., Reuben BG & Plotkin JS. Industrial Organic Chemicals. Wiley & Sons.

[5] Smith RB. (1959) "Kinetic Analysis of Naphtha Reforming with Platinum Catalyst." *Chemical Eng. Progress*, vol. 55, #6, pg. 76-80.

Ke-Min L, Hai-Yan G & Shi-Wei P. (2005) "A Study on Naphtha Catalytic Reforming Reactor Simulation & Analysis." *J. of Zhejiang University*, vol. 6B, iss. 6, pg. 590-596.

Reaction kinetics for alkane ("decane" proxy component) cracking are as follows: [5]

$$4.5C_{10}H_{22} + 4.5H_2 \rightarrow C_9H_{20} + C_8H_{18} + C_7H_{16} + C_6H_{14} + C_5H_{12} + C_4H_{10} + C_3H_8 + C_2H_6 + CH_4$$

$$rate = 3.6704*10^{21} e^{\frac{-287756.8}{8.314T}} P_{C_{10}H_{22}}$$

$$rate \equiv kmol/(m^3 hr), \qquad P \equiv MPa, \qquad T \equiv Kelvin$$

Reaction kinetics for cylcoalkane ("cyclohexane" proxy component) cyclization are as follows:[5]

$$C_6H_{12} + H_2 \rightarrow C_6H_{14}$$

$$rate = 3.33674*10^{19} e^{\frac{-275285.8}{8.314T}} P_{C_6H_{12}} P_{H_2} - 4.19816*10^{21} e^{\frac{-312237.9}{8.314T}} P_{C_6H_{12}}$$

$$rate \equiv kmol/(m^3 hr), \qquad P \equiv MPa, \qquad T \equiv Kelvin$$

Financial information

Cyclohexane represents complex naphtha cycloalkanes and n-decane represents complex naphtha paraffins. The linear alkane currently fractionates with diesel to earn **$0.98/liter** from Mr. Abbasi's facility. Cyclic hydrocarbons currently sell with gasoline for **$0.63/Liter** from Mr. Abbasi's facility (local Kurdish gasoline price, https://www.globalpetrolprices.com/Iraq/gasoline_prices/). The effective cost of local naphtha is **$0.325/Liter**. Sulfolane is **$5/kg**. "Benzene" product from the catalytic reformer is actually a mixture of Benzene, Toluene and Xylenes. Before sale this reformate mixture, commonly known as BTX, **must be separated to 99% purity**. The current benzene contract price is **$3.49/gal** for product brought to the world market by rail (https://www.icis.com/chemicals/channel-info-chemicals-a-z/). Xylene and Toluene command approximately **80%** of the benzene price. Product linear alkanes C5-C8 contribute to local gasoline sales. Linear alkanes >C8 contribute to local diesel sales. Hydrogen and hydrocarbons smaller than C_5 are consumed in facility operations for no credit. United States wages are **438%** higher than Iraqi salaries. Utility costs are listed below. MACR and straight line depreciation aligned with United States standards after regime change (2003). Regional taxes are **35%** (Iraqi control) or **15%** (Kurdish control). Minimally an economic analysis of crude oil feed K under Iraqi and Kurdish taxes is desired. Maximally, include complete economics for processesing either feed K or feed TQ1 *through the same facility* under both tax regimes.

Utilities entering battery limits of the proposed catalytic reformer.

	utilities
electricity	$0.25 kWhr
steam, 450 psig	$19.36/1000 kg
steam, 150 psig	$14.08/1000 kg
steam, 50 psig	$8.8/1000 kg
natural gas	$9.43/MMBTU
cooling water, 25^{o} C	$0.5/GJ

Environment, Health and Safety:

Environment, Health and Safety (EHS) aspects are critical to the economic viability, sustainability and social responsibility of chemical sector investment and operations. These aspects must be carefully considered during design to ensure that processes minimize raw feedstock consumption, safely contain process materials, and effectively treat potentially harmful discharges prior to environmental release.

These aspects are especially important when processes use or produce toxic and flammable materials. Thus, student designs will be judged through the lens of **Inherently Safer Design**, which integrates hazards amerlioration within design planning (https://www.csb.gov/videos/inherently-safer-the-future-of-risk-reduction/).

Inherently Safer Design

Atop a short description of Inherently Safer Design, student reports should desribe how the catalytic reformer plant and any associated innovations realize (or not) the principles of Inherently Safer Design. Namely, how does the student process incorporate (or not):

1. *Substitution (e.g. the use of less hazardous chemicals where possible)*

2. *Minimization (e.g. the reduction of stored chemicals and/or reactive & toxic chemical concentrations)*

3. *Moderation (e.g. the use of lower temperatures and/or pressures)*

4. *Simplification (e.g. reductions in process complexity to avert equipment failure)*

Student work should concisely and specifically name areas where facility design conforms to these principles and identify areas were design(s) might improve.

Process Safety Management Considerations[6]

Inherently Safer Design is related to, but not the same as, Process Safety Management (PSM). PSM is the use of multiple management systems to "keep chemical energy in the pipe" – a collection of considerations and interventations that prevent rare but catastrophic events that yield fires, explosions and toxic releases. This includes, but is not limited to, understanding the hazards of the process; conducting risk assessment; installing engineering and administrative controls such as alarms, interlocks, explosion and relief systems; and establishing management systems to ensure changes are managed, systems are maintained, and people know and follow procedures. Good engineers overcome the sprawling complexity of process design to communicate the details that inform potential catastrophy concisely and clearly to Operators, Maintenance Workers, Leaders, and Technical Staff.

1. **Process Hazards**
   Student designs must describe and recognize the hazards associated with potential human exposure to process materials, including raw materials, intermediate and finished products, by-products and wastes. To recognize hazards describe and compile a table of OSHA chemical exposure limits, NFPA diamond classifications, and lethal dose (LD_{50}) limits for process chemical constituents. This information is often found on *Safety Data Sheets* (SDS), formerly known as *Material Safety Data Sheets* MSDS. Screening for potential health risks is an important element of process safety that informs personnel protective equipment and standard operating protocols. Render protective reccomendations in the overall summary of this report's safety section.

2. **P&ID of the Major Fractionator**[7]
   You should assume that regulatory authorities require the application of *Best Available Control Technology (BACT)* to minimize gaseous and liquid wastes generated by a process. For illustration of best practice in your design, complete a detailed process and instrumentation diagram (P&ID) for the largest, by inventory, process distillation column (the "Major Fractionator").[8] The P&ID should include automatic controllers for pressure, level, and composition (temperature) management atop alarmed indicators for the detection of abnormal conditions. Describe the controls approach and size a pressure relief for this column assuming an onsite flare is available for the safe and complete combustion of vented material.

3. **Uncongested Vapor Cloud Deflaguration**[7]
   Student designs should consider relevant lessons learned from the industry, especially with respect to hydrocarbon explosions. To highlight extreme risks in hydrocarbons processing describe and perform a TNT equivalency calculation for the atmospheric

[6] https://www.aiche.org/ccps/resources/publications/books/guidelines-risk-based-process-safetyccps/documents/overview
[7] Crowl DA & Louvar JH Chemical Process Safety. Prentice Hall.
[8] Turton R et al. Analysis, Synthesis & Design of Chemical Processes. Prentice Hall.
Sloley AW (2000) "Effectively control column pressure." *Chemical Engineering Progress*. vol. 97, iss. 1, pg. 39-48.

detonation of all chemicals from the largest, by inventory, process distillation column (the "Major Fractionator"). For worst-case consideration assume all fractionator contents instantly and gaseously vent to atmosphere. Map the blast radius for damage to people and structures, an essential siting consideration for retrofit construction. Include a table of upper explosive limits (UEL) and lower explosive limits (LEL) to inform the installation of facility sensors and alarms. To mitigate risks, tabulate a "What-if" Hazards Analysis for the major fractionator.

Close the safety section with a discussion of discovered process hazards and best pracitces key to safe operation, information critical for facility operators and technicians.