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Problem-Based Learning on Incorporation of Data Analysis Skills into a Senior Course

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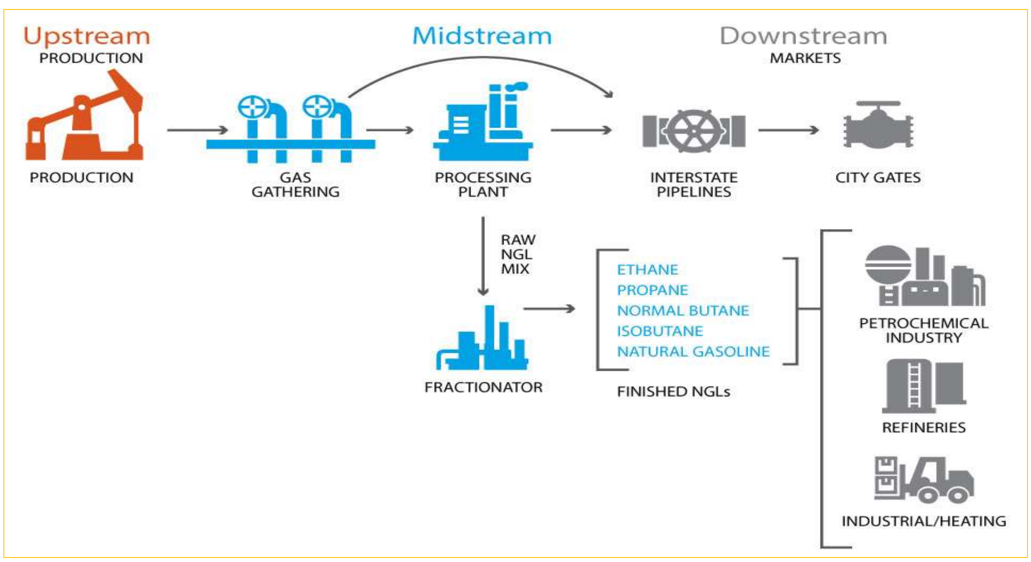

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Data → Sustainability

ChE + Data Skills

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ChE + Data Skills

Traditional ChE Skills

- Chemistry
- Thermodynamics
- Reaction kinetics
- Unit operations
- Process design
- Process control
- First-principles based process modeling

Data Skills

- Statistics
- Data preprocessing
- Feature engineering
- Representative ML algorithms
- Evaluation matrix
- Uncertainty
- Time series analysis
- Data analytics using spreadsheet/phython/R
- Basics of database management
- Data scraping and data crawling

https://www.linkedin.com/pulse/cheche-data-skills-compassion-helen-lou/?trackingId=OO9Zob42K62M8tfa0osuNA%3D%3D

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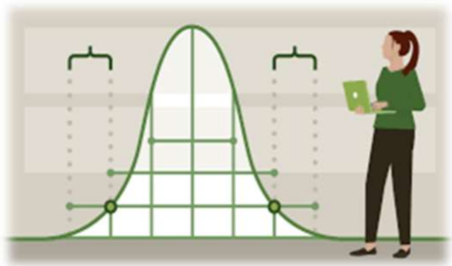
Data Skills

Spreadsheet is popular in the plants, and it is highly desirable for chemical engineering students to learn how to analyze data using an Excel spreadsheet



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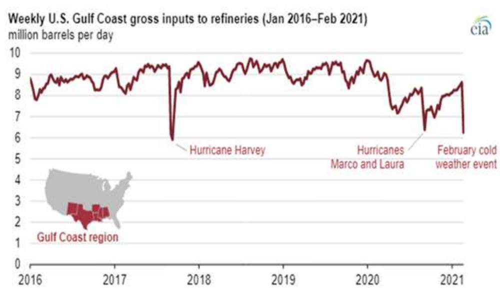
Data Skills

Chemical engineers should understand and be able to handle uncertainties in production



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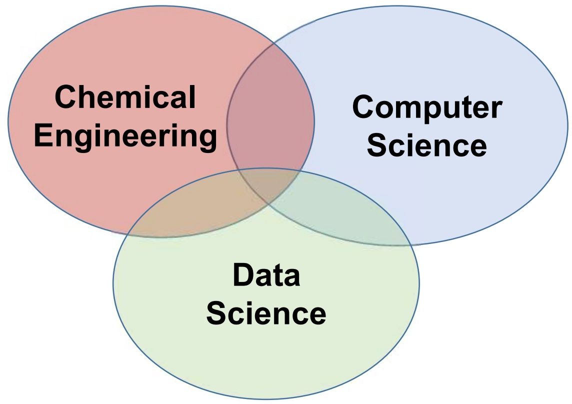
Combined Expertise for Success



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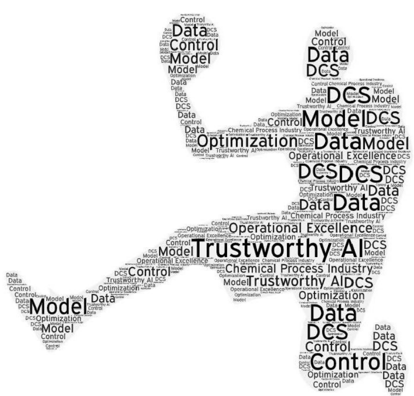
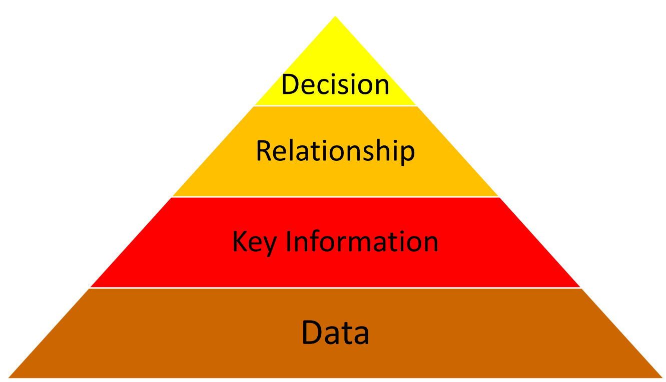
Using AI for Process Operational Excellence





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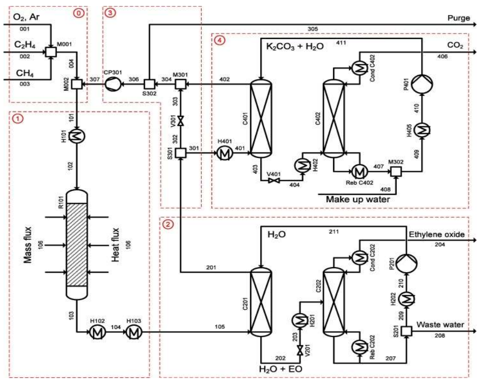
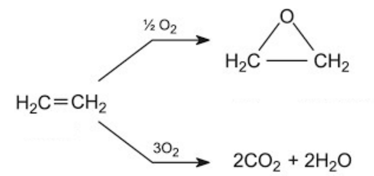
Example 1: An Ethylene Oxide Process





- **Selectivity improvement: >3%**
- **Annual Profit increase ($/yr): ~4.3 Million**

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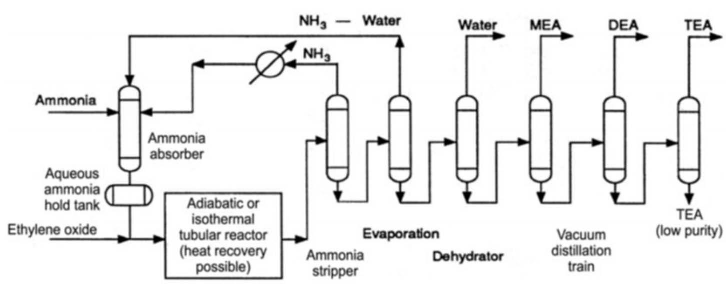
Example II: An Ethanolamines Process



MEA:Monoethanolamine
DEA: Diethanolamine
TEA: Triethanolamine

- **Reduce undesirable byproducts by 66%**
- **Save $0.3/lb**

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Example III: Combustion Modeling and Predictive Flare Control

Background: EPA Refinery Sector Rule (RSR)

- Destruction efficiency (DRE) ≥ 98% or
- Combustion efficiency (CE ≥ 96.5%)
- No visible smoke
- Pilot flame present all the time
- Combustion zone net heating value (NHVcz) ≥ 270 BTU/ft^3 on a 15-minute rolling average

Objective: Optimize the Flare Operating Parameters (steam/air injection rate and supplement fuel gas flowrate)

- Meet compliance of Combustion Efficiency (CE)/Destruction Efficiency (DRE) and opacity (no visible smoke)
- Minimize operating cost

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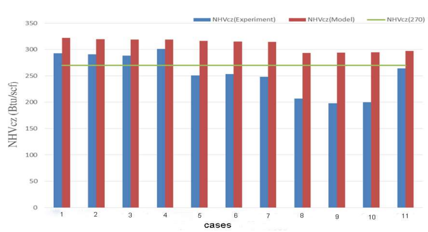
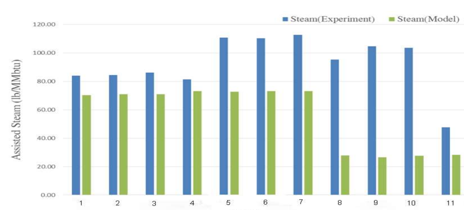
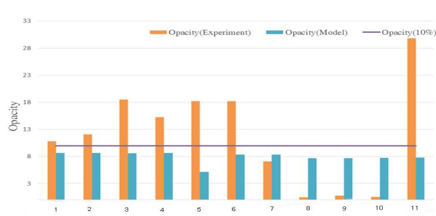
Optimized NHVcz vs. Historical Data



Optimized Assisted Steam vs. Historical Data



Optimized Opacity vs. Historical Data



Net cost saving:
Avg – 38.5%
Min – 16.0%
Max – 74.6%

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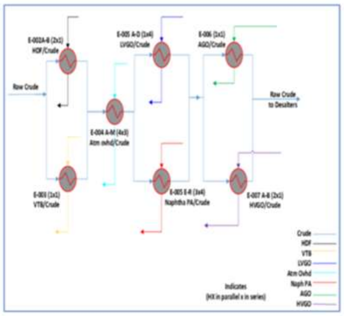
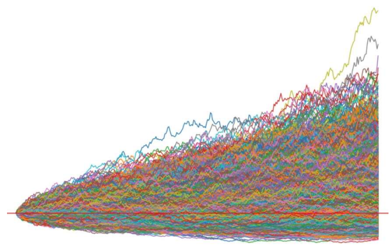
PBL: Refinery CDU Heat Exchangers Fouling Diagnosis





Monte Carlo Simulation

Lou, H. H., Y. Chen, and R. Singh, “Problem-Based Learning on Incorporation of Data Analysis Skills into Chemical Engineering Senior Advanced Analysis Course,” ***Smart and Sustainable Manufacturing Systems*** (March 2021), DOI: 10.1520/SSMS20200027.

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Closing the Skills Gap in the “Advanced Analysis” Course

- **Recap of basic statistics: this include how to describe the characteristics of a given data set using terms of mean, median, mode, standard error, standard deviation, sample variance, kurtosis and skewness, confidence level, etc.**
- **Identifying the outliers**
- **Correlation**
- **Regression**
- **Deal with uncertainty**
- **Time series analysis**
- **Optimization**

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Problem Based Learning (PBL) Approach

- **A student-centered approach**
- **Team work to solve open-ended problem**
- **Problem drives the motivation and learning**

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Skills Developed in PBL

- **Team work**
- **Managing projects and holding leadership roles**
- **Oral and written communication**
- **Self-awareness and evaluation of group processes**
- **Working independently**
- **Critical thinking and analysis**

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Monte Carlo Methods
Applications in Chemical Engineering

- **A statistical approach to provide approximate solutions to mathematically complex optimization or simulation problems faced with uncertainty by using random sequences of numbers.**
- **Monte Carlo simulations are used to model the probability of different outcomes in a process that cannot easily be predicted because of the intervention of random variables.**
- **In an application of asset reliability, heat exchanger performance was modeled considering manufacturing tolerances and uncertain flow distribution.**

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Case Study

- **Students introduced to**
  - **fundamentals of statistics**
  - **outlier detection using IQR**
  - **Monte Carlo simulation**
- **The students were divided into groups of 4–5 people each**
- **They were asked to figure out which heat exchangers in a refinery need to be cleaned with the help of Monte Carlo simulation and statistics analysis.**

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Case Study

- **Two years of related operation data from a crude distillation unit in a refinery**
- **The heat exchanger bank consists of seven counter current heat exchangers**
- **Raw crude on the tube side**

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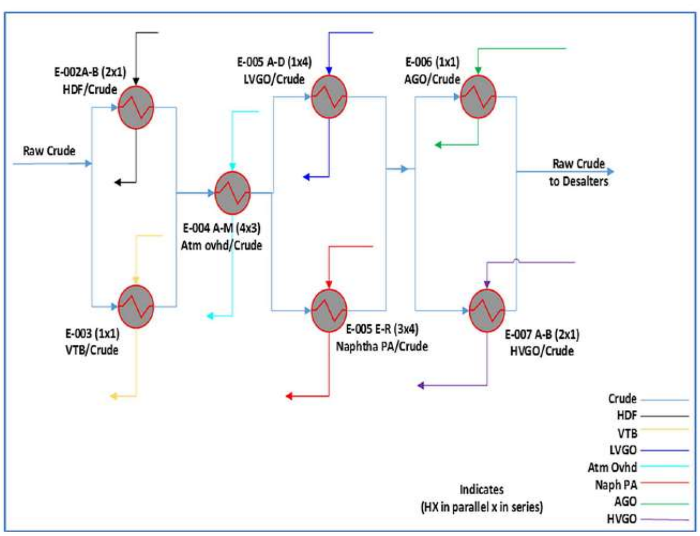
Schematic Flow of the Process



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Process Data

- **Flow rates, bph**
- **Crude densities, lb/ft^3**
- **Outlet and Inlet temperatures, F**
- **Exchanger area, ft^2**
- **Number of shells**
- **Heat capacity of the fluid, C_p**
- **Designed value of heat exchange rate, Q_{Design}**
- **Heat transfer coefficient during normal service, $U_{Service}$**

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Fundamental Equations

(1) LMTD = $\frac{[(T_{i1}\ To_2)-(T_{o1}\ Ti_2)]}{\ln[(T_{i1\_}To_2)-(T_{o1\_}Ti_2)]}$

Where:

T_{i1} = shell side inlet temperature,

T_{i2} = shell side outlet temperature,

T_{o1} = tube side inlet temperature, and

T_{o2} = tube side outlet temperature.

(2) $U_{values} = \frac{Q_{Design}}{A*LMTD}$

Where:

Q_{Design} = design value of heat exchange rate, and

A = heat exchange area.

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Sample of LMTD & HT Coeff Values

TABLE 1
Sample of LMTD and heat transfer coefficients values of E4

Design	LMTD	U (Actual)
5/1/2019	59	24.9
4/30/2019	59	24.9
4/29/2019	59	25.1
4/28/2019	58	25.5
4/27/2019	58	25.5
4/26/2019	56	26.1
4/25/2019	60	24.6
4/24/2019	61	24.3
4/23/2019	61	24.3
4/22/2019	58	25.5
4/21/2019	55	26.6
4/20/2019	53	27.9
4/19/2019	55	27.0
4/18/2019	58	25.4
4/17/2019	61	24.3
4/16/2019	59	24.9
4/15/2019	57	25.9
4/14/2019	57	25.7
4/13/2019	63	23.3
4/12/2019	60	24.4
4/11/2019	64	23.1
4/10/2019	63	23.5
4/9/2019	60	24.6
4/8/2019	61	24.0
4/7/2019	64	23.1
4/6/2019	63	23.4
4/5/2019	64	23.1
4/4/2019	63	23.4

Note: Highlighting indicates that the heat exchanger is functioning at or very near its U_{dirty} value.

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Sample of Process Data

TABLE 2
Sample of process data and some statistics data for a heat exchanger

	Raw Crude (Tube Side)		VTB (Shell Side)		Raw Crude (Tube Side)		VTB (Shell Side)		Area, ft²		
Design	Flow Rate, bph	Density, lb/ft³	Flow Rate, bph	Density, lb/ft³	Temp In, °F	Temp Out, °F	Temp In, °F	Temp Out, °F	LMTD	3,561	U (Actual)
11/21/2016	1,159.15	57.63	2,650.08	65.00	80	106	420	438	335	…	16.5
11/20/2016	1,195.13	57.66	2,464.41	65.00	82	108	440	459	354	…	15.6
11/19/2016	1,202.67	57.60	2,324.27	65.00	87	111	442	460	352	…	15.7
11/18/2016	1,207.68	57.69	2,323.83	65.00	90	114	444	462	351	…	15.7
11/17/2016	1,207.02	57.73	2,399.81	65.00	87	111	439	457	348	…	15.9
11/16/2016	1,165.46	57.52	2,332.02	65.00	87	111	439	458	349	…	15.8
11/15/2016	1,138.58	57.52	2,250.32	65.00	86	106	389	395	295	…	18.7
11/14/2016	1,170.74	57.52	1,989.48	65.00	85	105	371	373	277	…	19.9
11/13/2016	1,193.45	57.49	2,011.20	65.00	86	105	370	372	275	…	20.1
11/12/2016	1,146.68	57.52	1,979.28	65.00	85	102	369	370	276	…	20.0
11/11/2016	1,207.38	57.51	1,924.73	65.00	87	105	370	370	274	…	20.1
11/10/2016	1,254.88	57.71	2,002.22	65.00	88	111	369	366	268	…	20.6
11/9/2016	1,180.57	57.71	2,055.04	65.00	93	117	365	362	258	…	21.4
11/8/2016	1,080.05	57.71	1,675.12	65.00	95	130	358	345	238	…	23.2
11/7/2016	1,012.97	57.71	3,512.52	65.00	94	141	350	326	220	…	25.0
11/6/2016	885.88	57.71	…	65.00	88	114	274	256	164	…	33.6
Q1	2,285.31	56.45	2,030.81	65	80.73	100.36	384.43	382.95	288.33	…	…
Q3	3,552.83	57.41	2,370.57	65	93.82	109.06	396.45	399.01	302.74	…	…
IQR	1,267.52	0.95	339.76	0.001	13.08	8.70	12.01	16.06	14.41	…	…
Upper bound	5,454.11	58.85	2,880.23	65	113.46	122.11	414.48	423.11	324.37	…	…
Lower bound	384.03	55.01	1,521.16	65	61	87.31	366.41	358.85	266.71	…	…
Avg. (w/o outliers)	2,658.85	56.85	2,202.42	65	86.66	104.89	390.61	391.22	295.83	…	…
STD	868.25	0.55	256.31	0.01	7.88	6.91	8.60	12.32	10.17	…	…

Note: Avg. = average; STD = Standard Deviation; VTB = vacuum tower bottoms; w/o = without. Highlighting indicates that the heat exchanger is functioning at or very near its U_{dirty} value.

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Monte Carlo Simulation

TABLE 3
Monte Carlo simulation on E4

Monte Carlo RAND	LMTD	U (Calculated)
1	76.39	19.30
2	64.93	22.71
3	80.49	18.32
4	67.37	21.89
5	73.39	20.09
6	73.38	20.09
7	66.10	22.31
8	71.00	20.77
9	65.95	22.36
10	69.72	21.15
11	70.36	20.96
12	69.42	21.24
13	69.86	21.11
14	63.57	23.20
15	73.61	20.03
16	69.61	21.18
17	75.94	19.42
18	68.74	21.45
19	81.91	18.00
20	70.55	20.90
21	69.13	21.33
22	74.59	19.77
23	75.82	19.19

Note: RAND is a mathematical function in Microsoft Excel used to generate random numbers.

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Statistical Results of MC Simulation

Descriptive statistics of Monte Carlo simulation on E4

Descriptive Statistics	
Mean	20.73
Standard error	0.01
Median	20.64
Mode	#N/A
Standard deviation	1.42
Sample variance	2.01
Kurtosis	0.33
Skewness	0.44
Range	11.26
Minimum	16.09
Maximum	27.35
Sum	207,276.4
Count	10,000
Confidence level (95.0%)	0.03

Note: #N/A = Not Applicable.

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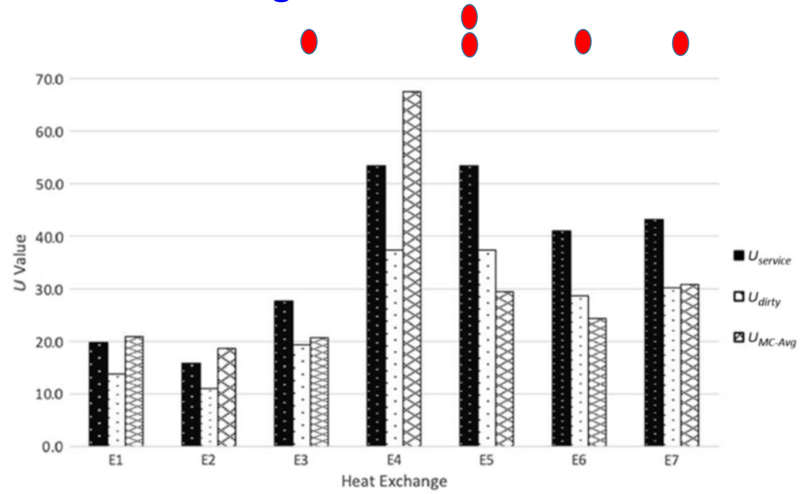
Cleaning Recommendations



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Cleaning Recommendations

TABLE 5
Cleaning recommendations/ranking for the heat exchangers

Exchangers	$U_{service}$	U_{dirty}	$U_{MC\text{-}Avg}$	Clean?	Rank
E1	19.8	13.9	21.0	No	5
E2	15.8	11.1	18.7	No	6
E3	27.7	19.4	20.7	Yes	3
E4	53.4	37.4	67.5	No	7
E5	53.4	37.4	29.5	Yes	1
E6	41.0	28.7	24.3	Yes	2
E7	43.2	30.2	30.9	Yes	4

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Discussion

- The calculated U values for each heat exchanger were compared with the design U value for each of the heat exchangers. If the calculated U value was 70 % less than the design U value, cleaning was recommended.
- It is possible that the U value might never meet the design U value, even after a full-service cleaning. This gives the engineer a better idea of what type of recommendation to make in terms of cleaning/servicing.
- Based on the data analysis of these heat exchangers, the students recommended which heat exchangers should be cleaned. The type of cleaning (shell only or both shell and bundle) can be determined through looking at the past maintenance history.

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Conclusion

- This project was well received by the students
- Some students eventually worked in the refineries as process engineers or maintenance engineers after graduation. This project helped them obtain some essential skills needed
- It is demonstrated that a PBL approach is highly effective for teaching data analytics.

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Thoughts

- Understand our customers - students
- Communicate with the industry
- Be adaptive
- Share the experience

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Acknowledgement

- Industrial partner
- Lamar University Center for Midstream Management and Science

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