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Quantitative and Qualitative Analysis of a Curriculum-Wide Chemical Process Project

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Abstract

The chemical engineering program at the University of California, San Diego has integrated a group project analyzing a chemical processing plant throughout the curriculum. The goal of the project is to tie together concepts in the core courses, which can otherwise appear disconnected. Students first analyze the chemical plant in Material and Energy Balances. They then build upon that analysis using the material they learn in Chemical Engineering Thermodynamics, Chemical Reaction Engineering, Separation Processes, Chemical Process Dynamics and Control, and, finally, in the capstone Chemical Plant and Process Design course.

This paper presents quantitative and qualitative survey results from students at different stages in the curriculum. A 5-point Likert scale was used to evaluate the students' perceptions of the connection between their courses and the impact of the group project on their learning outcomes. Taking an average value of the percentage of students who either "agreed" or "strongly agreed" across the 3 courses surveyed, 86% felt the project assignment helped them learn the course material, 83% felt working in a group helped them learn, and 80% recommended using the project again in the future. Most of the students in the two senior courses (72% and 82%) felt the project helped them understand the connection between their chemical engineering courses. In Material and Energy Balances, 95% of students felt the project helped them understand the connection between the topics taught within this first chemical engineering course.

The authors also coded responses to an open-ended question using thematic analysis and present the qualitative results here. This analysis identified that students appreciated applying their chemical engineering skills to real-world problems, were challenged by the project, enjoyed the project, and learned to work on a team. The thematic analysis also identified potential areas for improvement, such as assigning the project earlier in the quarter and having more accountability to ensure all students contribute equally to the project.

Introduction

The chemical engineering program at the University of California, San Diego has implemented a chemical processing plant group project throughout the chemical engineering curriculum. Four projects based on industrial chemical processes have been developed since 2012, with the project rotated every few years: (1) ammonia synthesis via the Haber-Bosch process, (2) vinyl chloride monomer synthesis from ethylene and chlorine, (3) methanol synthesis from natural gas, and (4) benzene synthesis via hydrodealkylation of toluene [1], [2]. The Haber-Bosch process for ammonia synthesis was assigned in the 2022-2023 and 2023-2024 academic years and is the focus of this publication.

These projects were designed to help students see the connections between their core chemical engineering courses, which can otherwise seem unrelated. Students synthesize the knowledge from their core courses during their capstone design project senior year. By adding the ammonia production plant project to 5 courses *before* capstone design, we aim to connect and integrate this knowledge earlier. By the time our students reach their capstone design courses, they have already analyzed a single chemical process from many angles. We hope this experience also makes their senior design project seem less daunting.

These group project assignments are also an instrumental tool to help students learn the course material. Compared to individual homework assignments which are assigned weekly throughout the quarter, we are comfortable assigning more challenging project questions, since students have additional time (~5 weeks) and resources (their *teammates* as well as office hours) to solve the projects. The many potential advantages of team work over individual learning have been well summarized by Felder *et al.* [3]: "cooperatively taught students tend to have better and longer information retention, higher grades, more highly developed critical thinking and problem-solving skills, more positive attitudes toward the subject and greater motivation to learn it, better interpersonal and communication skills, higher self-esteem, lower levels of anxiety about academics, and, if groups are truly heterogeneous, improved race and gender relations." Adding group projects in teams of 3-5 students early in the chemical engineering curriculum should improve student learning.

These projects also give students additional opportunities to develop their "ability to function effectively on a team" (ABET accreditation Criterion 3 Student Outcome 5 [4]). Passow [5] surveyed ~2000 engineering graduates in 11 engineering fields at 2 years, 6 years, and 10 years after graduation and asked them to rank the ABET competencies (a-k in 2012 [6]) in order of importance for engineering practice. Practicing engineers ranked *teamwork*, data analysis, *problem solving*, and *communication skills* as the *most important* competencies in their professional experience. These skills were ranked significantly above the other ABET competencies surveyed (math, science, and engineering skills, experimental design, process design, ethics, impact, life-long learning, engineering tools, and contemporary issues). More recent studies similarly emphasize the importance of teamwork skills [7] as well as a gap between the professional skills of recent engineering graduates and the expectations of employers [8, 9]. These studies suggest that more traditional coursework and individual assignments do not adequately address some of the most important skills for practicing engineers. These project assignments are designed to offer additional opportunities for students to develop teamwork skills, positioning them for success both in their capstone design courses and in their professional careers after graduation.

Methods: Curriculum-Wide Chemical Process Project

The Haber-Bosch process for ammonia synthesis was implemented in the courses indicated in bold in Table 1.

Table 1: The 14 required upper division chemical engineering courses (excluding electives) for a Bachelor of Science degree in Chemical Engineering at UC San Diego. Courses that incorporate the **chemical process project** are shown in **bold**. Laboratory and capstone courses where students *also work in teams* are *italicized*. **A)** A 3-year upper division chemical engineering course schedule is typically followed by students admitted freshman or sophomore year. **B)** A 2-year course schedule is typically followed by transfer students admitted junior year.

A)	Fall quarter	Winter quarter	Spring quarter
Sophomore Year	**Material and Energy Balances**	**Thermodynamics**	**Chemical Reaction Engineering**
Junior Year	Fluid Mechanics *Experimental Methods*	Heat Transfer Probability and Statistics	Mass Transfer
Senior Year	**Controls** **Separations**	**Chemical Plant and Process Design I** *Chemical Engineering Process Laboratory I*	*Chemical Plant and Process Design II* *Chemical Engineering Process Laboratory II*

B)	Fall quarter	Winter quarter	Spring quarter
Junior Year	**Material and Energy Balances** Fluid Mechanics	**Thermodynamics** Heat Transfer Probability and Statistics	**Chemical Reaction Engineering** Mass Transfer *Experimental Methods*
Senior Year	**Controls** **Separations**	**Chemical Plant and Process Design I** *Chemical Engineering Process Laboratory I*	*Chemical Plant and Process Design II* *Chemical Engineering Process Laboratory II*

The full Haber-Bosch process description and sample group project assignments for all courses are provided in Appendix A. A brief summary of each assignment is also described below. Students are typically provided with the background process description (Appendix A1) at the top of the project assignment for all courses. This includes a simplified process flow diagram for the industrial ammonia synthesis plant shown in Figure 1.

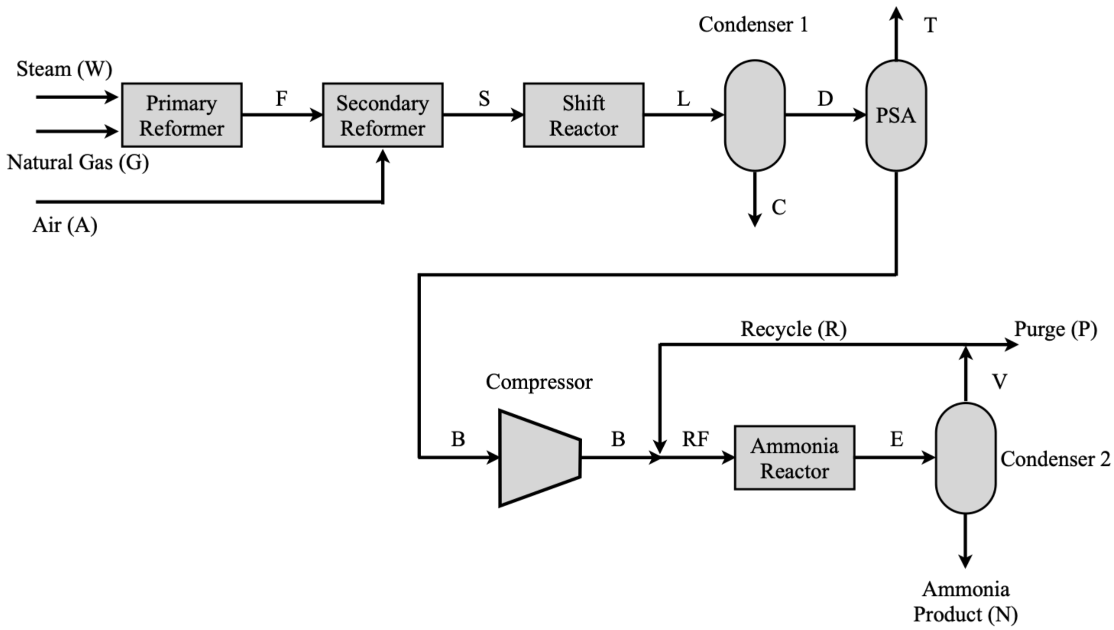

Figure 1: The process flow diagram students use to analyze the Haber-Bosch process for ammonia synthesis.

Students are first assigned the group project in their first core chemical engineering course: Material and Energy Balances (Appendix A2). Students apply their knowledge of material balance to solve for the composition and flow rates of all streams in the process. They evaluate the effect of recycle on conversion. They determine the amount of natural gas required for the reactor feed and to provide reactor heating. They perform some energy balance calculations, but perform most of the energy balance analysis the following quarter due to the time constraints of a 10-week quarter system. Students assume ideal gases, assume perfect separation occurs in the separators, and assume the reactors reach equilibrium.

The next quarter in Chemical Engineering Thermodynamics ("Thermodynamics"), the students are provided the same Haber-Bosch process background info (Appendix A1) along with new questions for the group project assignment (Appendix A3). They are also provided with an excel file containing the solution for all the stream flow rates and composition from the prior Material and Energy Balances project assignment. All students are therefore at the same starting point even if their solutions were incorrect or if they did not take Material and Energy Balances the prior quarter. Students then build upon their prior analysis by utilizing their knowledge of thermodynamics to determine the heating or cooling requirements for all process streams, reactors, and separators. They determine the work required by or recovered by all gas compression and expansion steps. They account for real gases, rather than assuming ideal gases throughout the process. They incorporate Henry's law to model the separator liquid streams more realistically. They still assume perfect removal of water/ammonia from the gas streams again due to time constraints, as flash calculations are not taught until the end of the 10-week quarter. They still assume the reactors reach equilibrium.

The following quarter in Chemical Reaction Engineering, the group project assignment focuses on the ammonia production chemical reactor (Appendix A4). Students no longer assume the reactor reaches equilibrium, but instead model the reaction kinetics of a packed-bed reactor. They incorporate heat exchanger design to model the reactor as a series of adiabatic packed-bed reactors with feed preheat and interstage cooling. They use Matlab to determine the molar flow rate, reactor temperature, and reactor pressure as a function of reactor length.

The project has not yet been expanded into the junior year course series Fluid Mechanics – Heat Transfer – Mass Transfer (Table 1), but the authors may incorporate the project into homework assignments in those courses in the future.

In the Fall quarter of their senior year, students simultaneously take Chemical Process Dynamics and Control ("Controls") and Separation Processes. For the Controls group project assignment (Appendix A5), the students design the temperature controller for the ammonia synthesis chemical reactor. Students analyze the dynamics of the reactor and develop optimum control parameters. They are given the transfer functions and analyze the process response, the open loop response, and the closed loop response. Students tune the relevant controllers and plot the controlled response.

In Separation Processes ("Separations"), the group project focuses on the two condensers used to separate water and ammonia (Appendix A6). The students use the chemical process simulation software Aspen Plus to accurately model these separation steps. They no longer assume ideal gases or ideal solution of liquids, but instead select an appropriate thermodynamic model to simulate the real fluid properties. They are tasked with selecting parameters to perform process optimization and analyzing the trade-off between recovery/purity and energy requirements. This ammonia synthesis project used only flash distillation, but other chemical process projects have also required students to select between and compare modeling of flash, distillation, absorption, and stripping columns for the separation train. The aim is to both increase their understanding of separation processes and introduce them to more open-ended problems without "correct" or "incorrect" answers. This should help prepare them for their capstone courses the following quarter, as well as real problems they will encounter in industry or graduate school after graduation.

In the Winter quarter of their senior year, the students analyze the Haber-Bosch process in their Chemical Plant and Process Design I course through individual homework assignments (Appendix A7). The last two quarters of their senior year, the students are already working in teams of four students on their capstone design project (which is not the Haber-Bosch process) and in their capstone unit operations laboratory courses. Instead of assigning additional teamwork, the Haber-Bosch process analysis is continued in individual homework assignments. Students develop process simulation skills in Aspen Plus by modeling the ammonia synthesis reactor-separator-recycle-purge loop and using Aspen's process optimization tools (sensitivity analysis and design spec) to optimize the process. They perform sizing calculations on the ammonia separator and determine the pressure vessel wall thickness. They also apply their knowledge of engineering economics to calculate the condenser capital cost and analyze the economics of the ammonia synthesis plant.

The project is currently not used in Spring quarter of the students' senior year, but the authors may incorporate it into homework assignments in Chemical Plant and Process Design II in the future. Specifically, analysis of the safety and environmental aspects of the process have not yet been included in the project and would be appropriate for this course.

The project was created by one of the authors of this publication, but the core courses are taught by many different professors in the department. Inclusion of the project each quarter is up to the course instructor's discretion. To encourage adoption, we provide the course instructors with the project assignment questions, project solutions, and grading rubric at the start of each quarter. Most instructors elect to assign the project, with a few exceptions. Instructors typically do not require the project when courses are offered over summer session due to the abbreviated course timeline. Instructors also did not require the project at the start of the COVID-19 pandemic when remote instruction made meeting to work on group projects more challenging.

While the format for these group project assignments is up to the course instructor's discretion and can therefore vary slightly, students are typically required to work in groups of 3 to 5 students. Students are allowed to select their own groups if they have preferred teams, with some students electing to instead be assigned to random groups by the course instructor. Students are not required to keep the same groups each quarter. The project is typically worth 10% of the overall course grade. This percentage was selected with the aim of being high enough to motivate students to take the project seriously, but low enough that final student course grades are still mostly evaluated on individual work (homework, quizzes, and exams).

Methods: Data Collection and Analysis

UC San Diego collects anonymous student feedback on teaching for all undergraduate courses at the end of each quarter. Instructors are allowed to add up to 5 custom questions to the standard question set. For the Fall 2023 quarter, the Haber-Bosch process project was assigned in Material and Energy Balances, Separations, and Controls. Student feedback was collected for all 3 courses.

For the senior year courses (Separations and Controls), questions 1) through 4) were asked using a 5-point Likert scale from "strongly disagree" to "strongly agree":

1) The group project assignment helped me understand the course content.
2) Working with the other members of my group on the group project assignment helped me understand the course content.
3) The group project assignment helped me understand the connection between the *concepts taught in this course and the concepts taught in my other chemical engineering courses*.
4) I would recommend using the group project for this course in the future.

Question 5) was added as an open-ended response question:

5) Is there anything else you would like to share about your experience with the group project? *Please indicate whether you were assigned the Haber-Bosch process for*

ammonia production in your courses last year or were first assigned this process for the Separations and Controls group projects.

For the first core chemical engineering course Material and Energy Balances, the same questions were used with two differences to Questions 3 and 5. The differences are highlighted in italics. Question 3 probed the connection between different concepts taught within the same course rather than the connection between courses. Question 5 was simplified since the students were seeing the project for the first time.

3) The group project assignment helped me understand the connection between *the different concepts taught in this course*.
5) Is there anything else you would like to share about your experience with the group project?

The qualitative data from question 5 was analyzed using the thematic coding process described in [10]. Responses such as "none" or "this was the first time I was assigned the Haber-Bosch process" that did not include any additional comments were excluded from the analysis, leaving 69 responses total. The two authors independently reviewed all 69 responses and came up with a list of themes or "codes". The authors then discussed and agreed upon one set of standard themes or "master codebook" to analyze the data. Both authors independently coded the data using the master codebook and discussed to resolve any discrepancies in the counting.

Results and Discussion

Table 2 shows the survey response statistics.

Table 2: The number of students enrolled and number of responses to the "strongly agree" to "strongly disagree" Likert-scale questions and open-ended "anything else to add about the project?" question is shown. The percent response rate for each class is calculated and shown in parenthesis.

Course	Number of students enrolled in course	Number of responses to Likert scale questions (% response rate)	Number of responses to open-ended question (% response rate)
Material and Energy Balances	113	101 (89%)	36 (32%)
Controls	99	87 (88%)	16 (16%)
Separations	97	87 (90%)	17 (18%)

For all 3 courses, approximately 90% of the students responded to the Likert-scale Questions 1) - 4). Fewer students (16%-32% of the class) also shared additional comments on the project in response to Question 5). Note that all 97 seniors enrolled in Separations in Fall 2023 were also enrolled in Controls, so the total number of students surveyed was 212 not 309 (99 seniors plus 113 sophomores or juniors). The authors chose to survey the seniors in both of their courses due to the different format of the projects in the senior courses. The Controls project had calculations more similar to traditional homework assignments with "correct" and "incorrect" answers. The

Separations project was more open-ended and focused on Aspen simulations more similar to a design project.

The response to the course project overall was very positive, as the majority of students in all three courses agreed or strongly agreed with all four of the statements posed in Questions 1) - 4) (Figures 2-5 and 7).

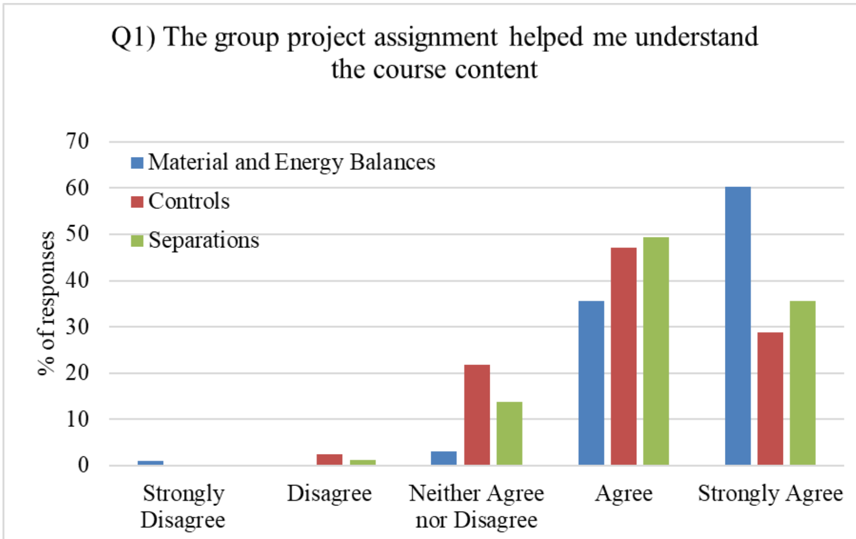

Figure 2: The percent of students who disagreed or agreed that the project assignment helped them understand the course content.

As shown in Figure 2, in the Material and Energy Balances course, 60% of the students strongly agreed and 36% of the students agreed that the group project assignment helped them understand the course content. Only 3% of the students were neutral (neither agreed nor disagreed), and only 1% (1 student out of 101 responding) felt it did not help them learn the course material.

For the senior year courses, the majority of students again agreed (47% and 49%) or strongly agreed (29% and 36%) that the project helped them understand the Controls or Separations course content, respectively (Figure 2). More students were neutral (neither agreed nor disagreed) for Controls (22%) and Separations (14%) than for Material and Energy Balances (3%). Again only a few students responded that it did not help them understand the Controls (2%) or Separations (1%) course content.

"Helped understand the course topics" was also identified as the most frequent theme in student responses to the open-ended question 5) ("Is there anything else you would like to share about your experience with the group project?"). This theme appeared in all 3 courses and appeared 18 times in the 69 total responses, including comments such as:

"It is a fun and interactive way to truly understand course material and to challenge the mind."

"The project was really enjoyable for me. It was challenging but solidified my understanding of the material."

"It made us really think about concepts we had learned in the class and put them into use."

These results are consistent with the results of a prior study of students assigned a similar vertically integrated design project at Pennsylvania State University [11]. Those students similarly ranked a case study project experienced throughout their curriculum as the most helpful tool for learning chemical engineering principles.

Figure 3 shows the responses for Question 2, which probed whether students felt that the group aspect of the project helped them learn the course material.

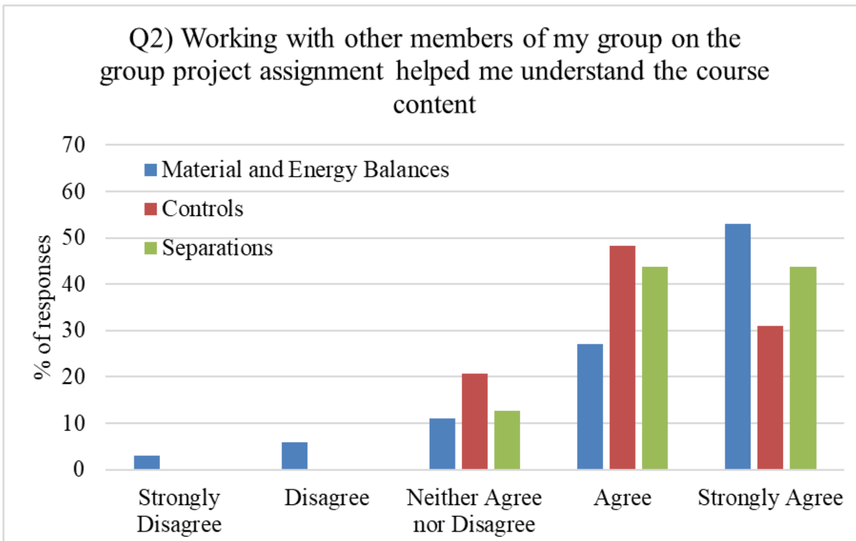

Figure 3: The percent of students who disagreed or agreed that working with their group members helped them understand the course content.

A majority of students agreed that working with other members of their group helped them learn the course material (Figure 3). 80% (Material and Energy Balances), 79% (Controls), and 87% (Separations) of students either agreed or strongly agreed with this statement. Only in Material and Energy Balances did any students disagree (6%) or strongly disagree (3%), but interestingly that course also had the highest percentage of "strongly agree" (53%). Two student comments addressed the benefits of collaborative learning:

"I felt like it really helped me to solidify my understanding of the concepts by allowing me to talk through the process in a group."

"Group project helped learn concepts I struggled with since I was working with peers."

Three additional themes related to the group aspect of the project were identified in the responses to Question 5). The theme "<u>learned to work on a team</u>" appeared 7 times, including:

"I think that the group project is a really good experience for us so that we could improve working together as a team which is definitely helpful for our career."

"I enjoy the group projects as it helped me learn how to work in a team and also apply the concepts we have learned in class to real life problems."

On the negative side, 7 student comments related to "challenging group dynamics" and 5 students said they "want more accountability". Most of these comments related to students feeling that members of the group did not contribute equally to the project:

"I wish there was more of a way that we can ensure everyone contributes in the group project or some sort of form to evaluate how we thought each group member did at the end of the project. Sometimes it feels like only a few members are contributing or you are just doing the whole project by yourself."

"Me and one other teammate ended up having to do most of the work for the project due to rest of the group constantly procrastinating on their part and/or or not knowing the course content enough to be able to solve the problems. I think it would have helped if there was a course of action where if some teammates were not doing their part despite being given chances to put in the work, they could be given a warning or some other incentive to contribute more equally to the project."

This issue of students not contributing equally is common in group projects [12]. The project statement attempts to address this problem by specifying that work should be divided equally, and the submission sheet requires students to identify which part of the project they contributed to (Appendix A1). However, no method for peer evaluation was incorporated into the project assignment or project grades in Fall 2023 when this survey was collected. Using peer evaluation methods such as CATME could improve this in the future [12], [13].

One of the goals of this project is to help students connect the concepts taught in their various chemical engineering core courses. Question 3 probed whether the project helped students see this connection (Figure 4).

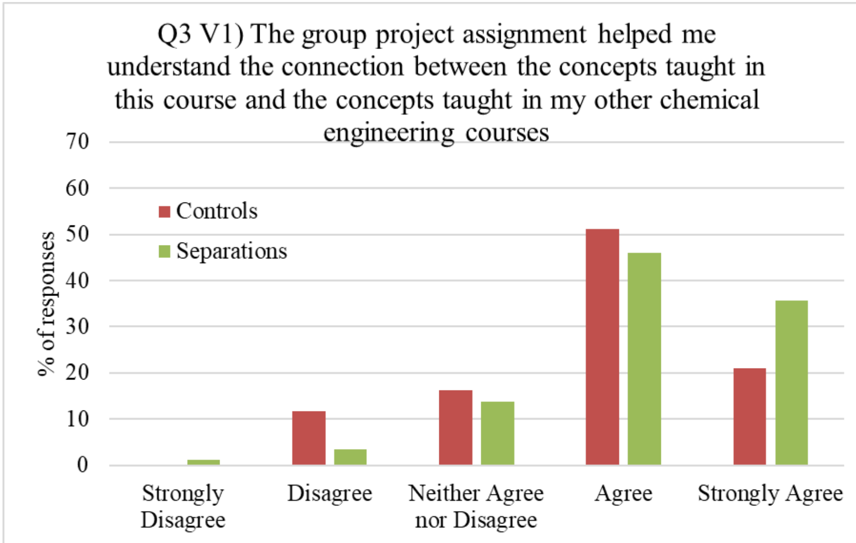

Figure 4: The percent of students who disagreed or agreed that the project helped them connect the concepts in their various chemical engineering courses.

The senior class surveyed in Fall 2023 was simultaneously assigned the Haber-Bosch project in Separations and Controls. As shown in Figure 4, the majority of students in Controls (72%) and Separations (82%) either agreed or strongly agreed that the project assignment helped them see the connection between these courses and their other chemical engineering courses.

These seniors consisted of two main cohorts with respect to the project assignments *prior* to Fall 2023, because the project topic was rotated between the 2021-2022 and 2022-2023 academic years. Approximately 30% of the seniors were enrolled in the Material and Energy Balances – Thermodynamics – Chemical Reaction Engineering series as juniors during the 2022-2023 academic year. This is the typical 2-year schedule for students transferring into chemical engineering from community college or another major junior year, as diagrammed in Table 1B). This cohort was assigned the Haber-Bosch process in all 3 of their courses junior year, making a total of 5 times they saw the *same* industrial chemical process. The second main cohort of students (~70% of the seniors) followed the typical 3-year upper division course schedule diagramed in Table 1A). These students were assigned a *different* chemical processing plant project, methanol synthesis for natural gas, during Material and Energy Balances in Fall 2021. As with many universities, UC San Diego switched to remote format at the start of Winter quarter 2022 due to a surge in COVID-19 cases. Due to the extra challenge of meeting with groups during remote learning, this cohort was not assigned the group project in Thermodynamics or Chemical Reaction Engineering. So this cohort analyzed a chemical process project 3 times in total, but the Haber-Bosch process only twice.

Many students who provided comments on the project did not indicate whether or not they had been assigned the Haber-Bosch process in a previous course. The survey responses collected by UC San Diego are also anonymous. Therefore, while it would have been interesting to compare the results of Question 3 between these two cohorts of students, the anonymous survey format made this impossible.

Material and Energy Balances is the first upper division chemical engineering course and the first time the students are assigned the course project. Therefore, for this course, the question instead asked whether the project helped students connect the various concepts *within that course*. The results are shown in Figure 5.

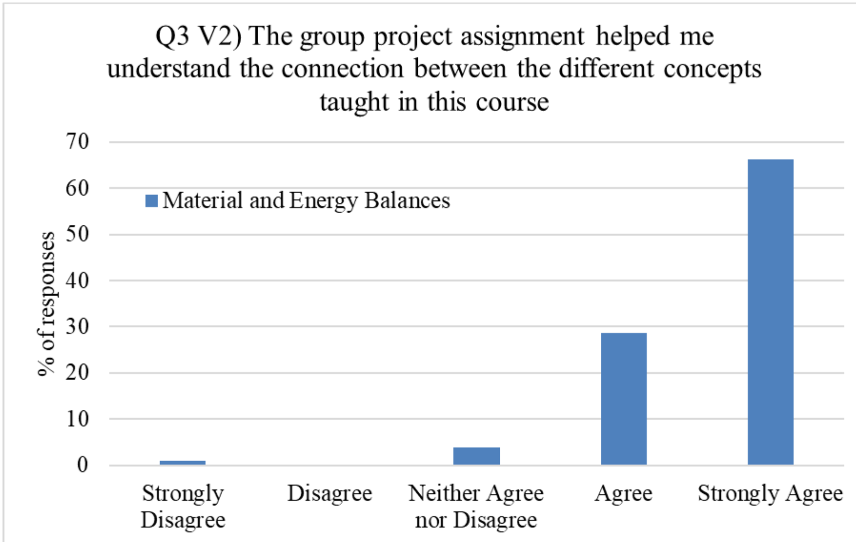

Figure 5: The percent of students who disagreed or agreed that the project helped them connect the different concepts taught within the Material and Energy Balances course.

Most students strongly agreed (66%) or agreed (29%) that the group project helped them understand the connection between the different concepts taught in Material and Energy Balances. "Helped connect course concepts" was also identified as a theme in the open-ended responses with comments such as:

"I like the group project because it makes you connect all the topics you learned."

"The group project definitely kept me engaged and helped my group realize the connections and overlaps of our course content, but it took a decent amount of time that interfered with our other classes."

Figure 6 shows additional themes identified from the open-ended response question. All themes appearing 3 or more times and in more than 1 course are shown.

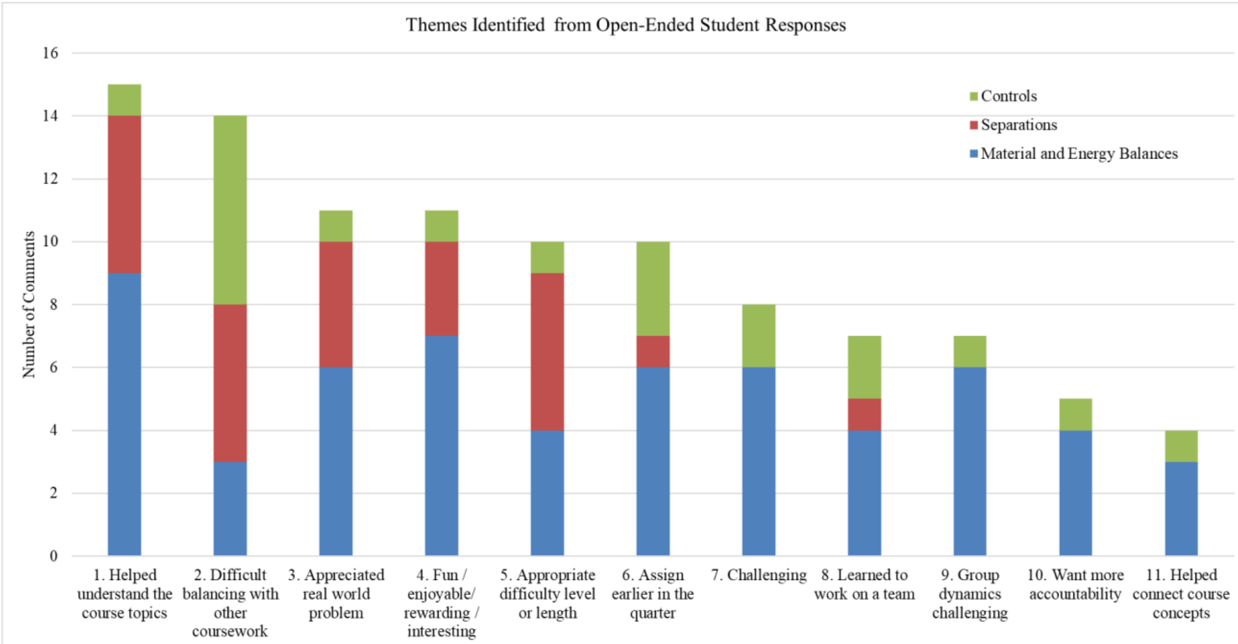

Figure 6: All themes that appeared in 3 or more student comments and in more than 1 course, by frequency.

The most frequent theme "helped understand the course topics" was already discussed above, as was theme 8 "learned to work on a team" and theme 11 "helped connect course concepts".

The 3rd most common theme, appearing 11 times, was that students enjoyed applying their knowledge to "real world problems". 11 students also commented that the project was either "fun, enjoyable, rewarding, or interesting".

"Overall, this project was a helpful way to visualize how this process operates in the real world and the costs that it entails."

"I really enjoyed it because it introduced us to real chemical engineering applications. The data collection from ASPEN and analysis was also helpful since it gave us an understanding of what a chemical engineer does in industry."

"It was fun approaching a challenging project with new friends."

"It actually felt very rewarding to complete the problems and find the answers."

The word "challenging" was used to describe the project 8 times, but often in a positive context in explaining how it helped the students learn. Below are some examples:

"The group project was definitely challenging, but at the same time, I could definitely see the class's applications to a real process and helped cement understanding of the material."

"I think that, for the most part, the group project is a great way to see what chemical engineering is about while also helping us learn by giving us more challenging problems."

Another common theme was that the project assignment was the "appropriate difficulty level or length", which appeared 10 times between the 3 courses.

"It was the right amount of difficulty for a group."

"The project is an appropriate length."

A few additional themes were identified in only 1 course. In Controls, "too long or too overwhelming" was mentioned 3 times. In Separations, 3 students expressed "appreciation for Aspen" process simulation software. For Material and Energy Balances, 4 students said they "appreciated office hour help" and the ability to check solutions. In that course, the instructor viewed the project as a tool to facilitate learning the course material rather than as a tool to test the course material knowledge. The students were therefore encouraged to start the project early and come to office hours to check their answers along the way, so that they could identify, learn from, and correct any mistakes.

"The project has been a lot of work but it is a lot of fun. I appreciate that the professor and instructional assistant were willing to check our answers to the project. This made it a lot less daunting and really helped my understanding of the material."

The second most frequent theme, appearing 14 times in the 69 responses, was "difficult to balance with other coursework". This was often mentioned along with the theme "assign earlier in the quarter".

"It's a bit hard juggling weekly homeworks and quizzes and projects and studying."

"The worst time to release the project is in the later half of the quarter. Multiple projects, homework assignments, AND quizzes was very overwhelming with such limited time."

"I felt that the project could have been assigned to us a bit sooner just because it felt like a time crunch towards the end. Although we did not have the skills to solve some of the problems in the material balance section, assigning it to us earlier would give us a chance to look at the questions and understand how to apply the concepts we learned in class on the project and we would have more time to check our work."

The project is typically assigned about halfway through the quarter once students have learned enough of the course material to make good progress on it, although in the Fall 2023 quarter it was assigned towards the end of the quarter for the senior courses. The comments demonstrate that for future courses, assigning the project as early as possible would be beneficial for the students. However, there is a balance because assigning the project too early could result in confusion if the students do not have enough knowledge to make progress. The authors recommend assigning the project early but updating students frequently on which questions have or have not already been covered in the lecture material so students know which problems can be solved.

The two other negative themes "group dynamics challenging" and "want more accountability" were already discussed above, with suggestions for improvement such as incorporating peer evaluations for future years.

Finally, Figure 7 shows that for all 3 courses, the majority of students recommend using the project for future courses. Taking an average of the percentages for all 3 courses, 80% of students agreed or strongly agreed that the project should be used again in the future and 16% were neutral. Only a very small percentage of students (4%) recommended against using the group project in the future.

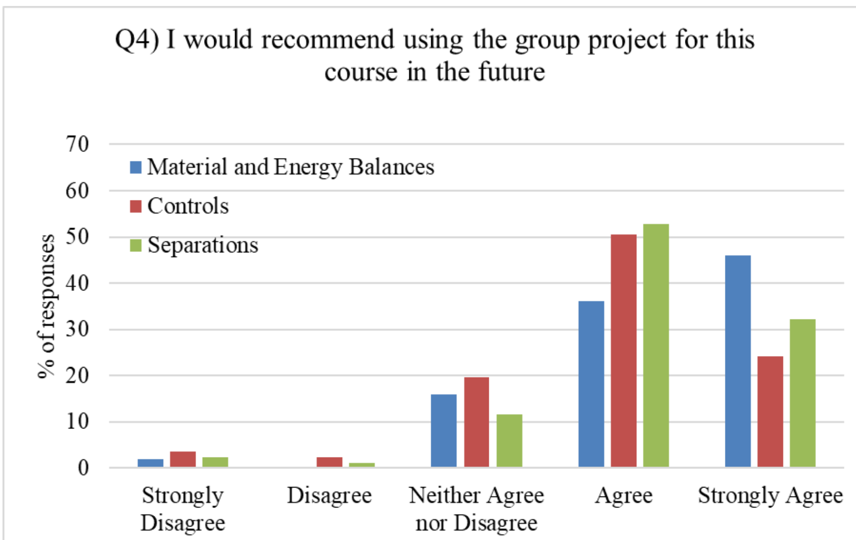

Figure 7: The percent of students who disagreed or agreed that the project should be used in future courses.

For all 4 Likert-scale questions (Figures 2-5 and 7), while all 3 courses had very positive responses, the Material and Energy Balances course had even more "strongly agree" responses than the 2 senior year projects. This could be due to a difference in the assignment content. We also noted more frequent comments with the theme "difficult balancing with other coursework" from the seniors who were assigned 2 projects the same quarter, so this may have affected their recommendation of the project. By senior year, many students have also already made connections and formed study groups with other students in their major (possibly in their prior course projects). The positive effects of collaborative learning from the group project may be most beneficial in the student's first upper division chemical engineering course.

A limitation of this research is that it is based on self-reported responses only. No attempt was made to directly measure a difference in student learning outcomes or teamwork skills with versus without the course project. Dividing students into two cohorts and quantitating statistically significant differences in their learning or attributes while also controlling for other variables such as instructor differences is challenging. For the senior class evaluated in this publication, there were two cohorts of students who were assigned the Haber-Bosch process project in either 2 or 5 courses, as discussed previously. The authors considered attempting a comparison of student learning outcomes between these two cohorts. However, deconvoluting the effects of the project alone versus other confounding variables (remote instruction versus in-person learning for core courses, transfer versus 4-year students, and instructor differences) would not have been possible. Given the overwhelmingly positive student response to the projects, the authors have no plans to remove the project from the curriculum in the future to perform such a comparison, as doing so may negatively impact the cohort not assigned the group project. A more extensive survey of the cohort of students completing the project in all 6 courses, however, is a subject of ongoing research.

Conclusions

By incorporating one industrial chemical process into group projects throughout the curriculum, students at UC San Diego analyze a single chemical process from almost every aspect. Students determine the stream composition and flow rates in Material and Energy Balances. They calculate the process energy requirements in Thermodynamics. Students focus on the chemical reactor to model the reaction kinetics in Reactor Engineering and to design a control system in Controls. They focus on modeling the process separation steps in Separations. Students learn new process simulation tools and determine equipment sizing and capital costs in Chemical Plant and Process Design I.

Based on student comments from surveys in 3 of these courses, students enjoyed working on the projects, were challenged by it, appreciated that it provided them with a real-world application, and felt it helped them learn to work together as a team. Student comments suggested the project could be improved by incorporating a peer evaluation system to increase accountability within the groups and by assigning the project earlier in the quarter to give more time to work on it.

The quantitative results of the student survey responses to the project were overwhelmingly positive. The results suggest that the project was very effective at helping students connect chemical engineering concepts within or between courses. Taking an average for the 3 courses surveyed, 86% of students believed the project assignment helped them learn the course material, 83% of students felt that working in a group helped them learn the course content, and 80% recommended using the project again in the future.

Acknowledgement

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Appendix A1. ***Chemical Process Project Description and Background*****. Plant for Production of Ammonia: Haber-Bosch Process**

<u>Introduction and History:</u>

One of the most critical nutrients for plant growth is nitrogen. Unfortunately, in its most common, atmospheric form, diatomic nitrogen cannot be readily utilized by plants. It is for this reason that fertilizers with a large quantity of nitrogen-rich compounds are used for agricultural purposes. For most of human history, the only available fertilizer sources were from the leavings of animals. With the industrial revolution, there was a need for a massive increase in agricultural production, hence a need for more nitrogen nutrients. For most the 1800s, Peru, Bolivia, and Chile provided the world with nutrients for fertilizers thanks to their exclusive ownership of high-quality guano and saltpeter deposits. However, this still did not provide enough nitrogen-based compounds for world demand in the areas of agriculture and explosive materials.

In the early 20th century, significant scientific research was performed to produce ammonia on an industrial scale. Ammonia serves as the general precursor for the production of most nitrogen-containing materials. In the first decades of the 1900s, Fritz Haber determined the chemistry and reaction conditions to produce ammonia, while Carl Bosch developed the process to produce it on an industrial scale. Perhaps one of the greatest discoveries in the 20th century, both earned Nobel prizes for the development of the Haber-Bosch process.

It cannot be emphasized enough the importance of this process. The ability to mass-produce ammonia (and hence to industrialize agriculture) was directly responsible for the growth of the world population by six billion people over the past century. Today, ammonia produced by this process sustains one-third of the Earth's population. Half the protein in humans contains nitrogen that was originally fixed by this process. Approximately half a billion tons of ammonia is produced each year by the Haber-Bosch process. This can be extremely energy intensive, consuming as much as 5% of the world's natural gas production and 1-2% of the world's annual energy supply. For this reason, and due to potential environmental dangers, an ammonia plant must be designed carefully, accounting for all material and energy needs.

References: ISBN 0-262-19449-X [14], ISBN 978-0-307-35178-4 [15], ISBN 0-8155-0734-8 [16]

<u>Process Description:</u>

Ammonia synthesis plants have been in operation since World War I, and there are many alternative designs available for such plants. However, we will analyze the structure provided. Crude natural gas is first desulfurized to produce the feedstock to the plant with the composition provided in the table below. This feed gas is then processed through a multi-stage reactor/separation sequence with water and air to produce N_2 and H_2 in exact stoichiometric proportions. These feed gases are then compressed to extremely high pressure and reacted over Fe-based catalysts to produce ammonia. After condensing this ammonia out, most of the unreacted feed gases are recycled to increase product yield.

Component	Mole %
Methane	91.6
Ethane	5.9
Propane	0.6
Butane	0.1
Carbon Dioxide	1.8

Steam Reforming:

- Primary Reformer -

Natural gas is traditionally reformed to yield CO and CO_2 via reforming and water-gas shift reactions:

Reforming (R1): $$C_nH_{2n+2} + nH_2O \leftrightarrow nCO + (2n+1)H_2 \quad (1)$$

Water-Gas Shift (WGS): $$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (2)$$

These reactions are usually conducted over a Ni-based catalyst. In our system, the reactor operates at P = 35 bar and T = 760 ºC. The reactions for ethane, propane, and butane go to completion. However, methane reforming and WGS go to equilibrium. The water to carbon feed ratio is 2.5:1. The water is provided by a nearby lake at 25ºC. Prior to entering the reformer, the water is vaporized, and both streams combined are pre-heated and compressed.

The heat for the reformer is provided by combustion (externally) of additional natural gas with excess air.

Combustion: $$C_nH_{2n+2} + \frac{3n+1}{2}O_2 \rightarrow nCO_2 + (n+1)H_2O \quad (3)$$

- Secondary Reformer -

Since a moderate amount of methane is still present in the gas mixture, the mixture is further reformed at higher temperature to drive equilibrium higher. Preheated air is reacted with methane to provide N_2 to the system as well as produce more H_2.

Secondary Reforming (R2): $$CH_4 + \frac{1}{2}O_2 \rightarrow CO + 2H_2 \quad (4)$$

This reactor uses a different Ni-based catalyst and operates at 1000ºC and 35 bar. All oxygen is consumed.

- Shift Reactor & Pressure-Swing Adsorption (PSA) -

CO and CO_2 are poisons for the ammonia synthesis catalyst, so they must both be removed. Direct condensation is not an option since the necessary temperatures would result in N_2 condensation as well. Thus, a different route is taken. First, a shift reactor is used to convert most the CO to CO_2 via the Water-Gas Shift (WGS) reaction, as shown above. In this reactor, an iron oxide/ chromium oxide catalyst is used at 300ºC and 35 bar.

The exhaust gas is then cooled and all the excess steam is removed. This dry gas is then sent through a chemical adsorption process, known as Pressure-Swing Adsorption (PSA). The details of the process are too complicated for this course, but ultimately it removes most of the CO_2 from the process stream. Residual CO_2 at this point is generally approximately 1000 ppm.

- Methanantion Reactor -

Even minute amounts of CO and CO_2 will destroy the ammonia reactor catalyst so the remaining amount of each is converted back into methane via the following reactions:

Methanation of CO (M1): $$CO + 3H_2 \rightarrow CH_4 + H_2O \tag{5}$$

Methanation of CO_2 (M2): $$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \tag{6}$$

Another Ni-based catalyst is used and operating conditions are typically about 300ºC and 25 bar. The only form of carbon in the exhaust is methane. Subsequently, the stream is sent through another condenser to remove all remaining water. At this point, only CH_4, H_2, and N_2 are present - the latter two in a 3:1 ratio.

Note: for simplification in this project, it will be assumed that the PSA removes ALL remaining CO and CO_2. Hence, no methanation reactor or condenser is necessary at this point.

Ammonia (NH_3) Synthesis:

- Ammonia Reactor -

After the purification steps, the reactants are compressed to an extremely high pressure of 175 bar and mixed with a very large recycle stream. This reactor feed is then heated to 1000ºF and reacted isothermally over an Fe-based catalyst. In a single-pass, only 20-30% conversion is typically obtained, hence requiring significant recycle. The catalyst is inactive at lower temperatures, but equilibrium is severely reduced at higher temperatures, so a mid-range temperature is chosen. The pressure is also limited because operation at these high pressures can be dangerous and requires expensive, specialized equipment.

Ammonia Synthesis (NS): $$N_2 + 3H_2 \leftrightarrow 2NH_3 \tag{7}$$

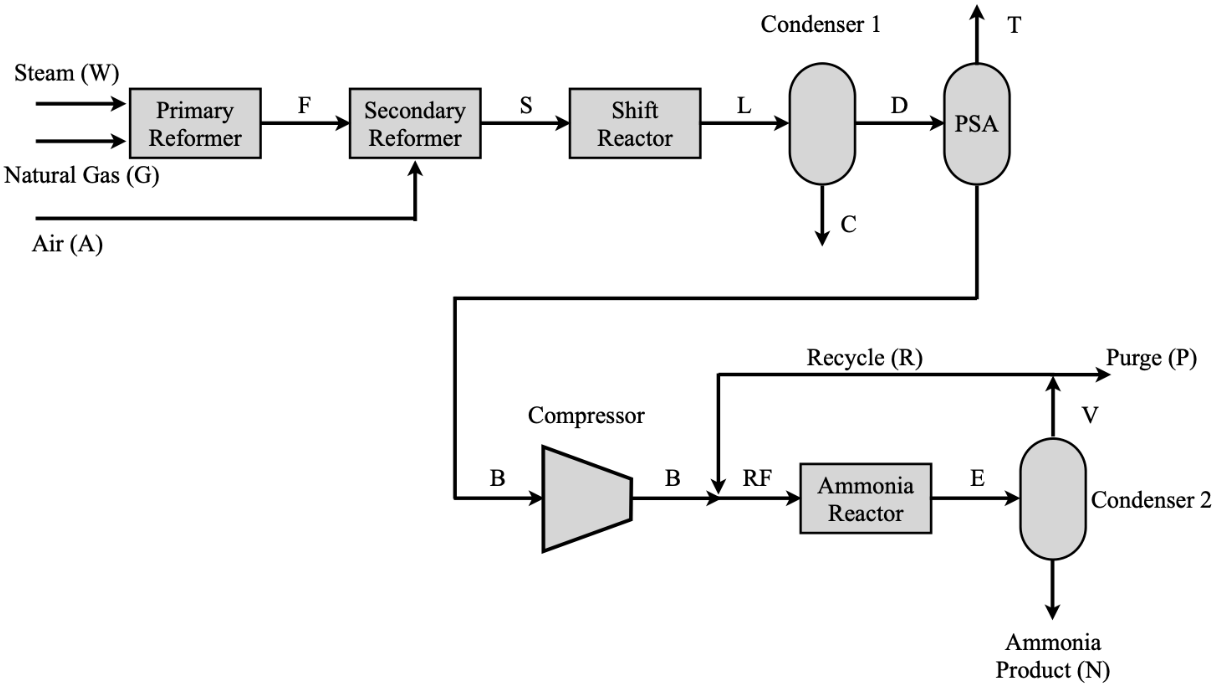
- Separation and Recycle -

After the reactor, the exhaust is cooled in a condenser to remove all the ammonia as a liquid. Since ammonia condensers rarely operate above 10 bar, the stream is expanded in a turbine first. To offset the accumulation of inert gases in this reactor, a purge stream is also required. 99% of the vapors leaving the condenser are recycled while the rest is purged. The recycle stream is compressed back to 175 bar before being mixed with the PSA exit stream (stream B).

Energy Considerations:

Energy integration is of key importance in modern ammonia synthesis plants. Students will be asked to determine various energy/work requirements throughout the process.

Process Flow Diagram:



Note: Stream labels are provided in the diagram.

See the following pages for the plant design and a list of specific design features.

Groups:
You are allowed to work on this project in groups of 3 to 5 students. Groups CANNOT be any larger. Also, NO ONE can work alone. This is supposed to be a collaborative effort, so you have to find fellow engineers to work with. All group members are expected to contribute equally and the work provided should label clearly which person contributed to what parts. Each group is expected to turn in a single completed project.

Worth: 10% of the overall course grade. DO NOT WAIT UNTIL THE LAST MINUTE TO START THIS PROJECT. YOU WILL REGRET IT.

Appendix A2. Sample Group Project Assignment for *Material and Energy Balances*

(Haber-Bosch process for ammonia synthesis Introduction and History, Process Description, and Process Flow Diagram sections are provided in Appendix A1.)

Your Assignment:

Analyze the provided plant design to determine the amount of ammonia product that can be produced under the conditions provided. You will utilize material and energy balances, as learned in this course, to determine flow rates, concentrations, and heat/work requirements throughout the process. Our goal is to determine various operating conditions and whether the current setup of the plant will be profitable.

Project Goal:

The purpose of this project is to introduce you to a complete process in a chemical plant and tie together all the concepts taught in Material and Energy Balances. You will determine how this plant operates under idealized conditions (ideal reactors ignoring kinetics, ideal separation units, ideal gases, etc.). You will be re-introduced to this project throughout your curriculum in Chemical Engineering at UC San Diego to correct these simplified assumptions and model this plant more accurately.

Process Design Features:

(1) For every mole of carbon in the natural gas feed, 2.5 moles of water are fed in the steam feed.

(2) The water is provided by a nearby lake at 25ºC and 1 atm. Both the water and natural gas feed streams start at 25ºC and 1 atm, but are pre-heated to 600ºC then isothermally compressed to 35 bar.

(3) The primary reformer operates at 760ºC and 35 bar.

(4) All ethane, propane, and butane are consumed in the primary reformer.

(5) The methane reforming and WGS reactions are equilibrium limited. The equilibrium relations are as follows:

$$K_{R1,CH4} = \frac{p_{CO}p_{H2}^3}{p_{CH4}p_{H2O}} \qquad \log(K_{R1,CH4}) = \frac{-11{,}769}{T(K)} + 13.1927$$

$$K_{WGS} = \frac{p_{CO2}p_{H2}}{p_{CO}p_{H2O}} \qquad \log(K_{WGS}) = \frac{1197.8}{T(K)} - 1.6485$$

where partial pressure p_i is defined as the mole fraction of species i times the total system pressure, $p_i = y_i P$.

(6) The furnace (to heat the primary reformer) is fed natural gas and 25% excess air at 1 atm and 25ºC, and the effluent gases leave at 900ºC.

(7) Air is pre-heated to 600ºC before entering the secondary reformer. The flowrate of A is set such that 100% of the oxygen is consumed in the reactor.

(8) The secondary reformer operates at 1000ºC and 35 bar.

(9) Stream S goes through a heat exchanger and is cooled to 400ºC before entering the shift reactor.

(10) The shift reactor operates at 300ºC and 35 bar. The reaction goes to equilibrium as defined by the WGS equilibrium above in Feature #5.
(11) In Condenser #1, only water is removed from L and stream D is water-free.
(12) In the PSA, all CO and CO_2 are removed and leave in stream T.
(13) In streams B, RF, E, V, R, and P, the ratio of H_2:N_2 is constant at 3:1. Note, there may be other compounds (inerts) still present.
(14) Stream B passes through a compressor where the pressure is increased from 35 bar to 175 bar adiabatically. The exit volumetric flow rate is 1/3 x the inlet flow rate.
(15) At the mixing point, streams B and R mix to some intermediate temperature. Stream RF is then heated to 1000ºF before entering the isothermal ammonia reactor.
(16) The ammonia reactor operates at 1000ºF and 175 bar and goes to equilibrium. The equilibrium relations are as follows:

$$K_{NH3} = \frac{p_{NH3}^2}{p_{N2} p_{H2}^3} \qquad \log(K_{NH3}) = \frac{3629.3}{T(K)} - 8.9596$$

where partial pressure p_i is defined as the mole fraction of species i times the total system pressure, $p_i = y_i P$.
(17) The ammonia reactor exhaust (stream E) passes through an adiabatic turbine to recover work and decompress the gas stream to 7 bar. The volumetric flowrate out of the turbine is 11 x the flowrate in.
(18) The condenser cools the turbine exit stream to 0ºC to condenses all ammonia out of stream E and into stream N (the final product).
(19) Of all the vapors in stream V, 99% is recycled into stream R, while the remainder is purged in stream P.
(20) Finally, the vapors in stream R are adiabatically compressed back to 175 bar before mixing with stream B. The volumetric flowrate out of the compressor is 10% of the inlet flowrate.
(21) <u>ALL VAPORS CAN BE TREATED AS IDEAL GASES</u>.

<u>Process Question (to be completed in teams of 3-5 students):</u>

Part 1 - Material Balance Questions: Let G = 100 mol/s unless stated otherwise

1. (a.) What is the conversion of the CH_4 in the primary reformer?
   (b.) What fraction of the hydrocarbon feed remains after the primary reformer (in stream F)?
2. (a.) How much air is needed for the secondary reformer?
   (b.) What is the conversion of the CH_4 in the secondary reformer?
   (c.) What fraction of the original hydrocarbon feed remains after the secondary reformer (in stream S)? *(Note: Q2 and Q3 may not be able to be solved independently.)*
3. (a.) What is the conversion of CO in the shift reactor?
   (b.) What is the composition of stream L in mole fraction (before the stream is separated)? *(Note: Q2 and Q3 may not be able to be solved independently.)*
4. What % of the original water fed (stream W) is removed from Condenser 1 in stream C?
5. After the PSA step, what is the composition and flow-rate of:
   (a.) the carbon-rich stream (T);
   (b.) the ammonia synthesis feed stream (B)?

6. (a.) Are there inerts in the ammonia section (bottom half) of the plant? If so, what are they?
   (b.) What is the composition (molar flow rates and mole %) of streams B, R, and RF?
7. (a.) What is the single-pass conversion of N_2 (or H_2) in the ammonia reactor?
   (b.) What is the overall conversion of N_2 (or H_2) in the ammonia reactor?
8. (a.) For 100 mol/s of natural gas feed, how much ammonia is produced?
   (b.) If the plant must produce 10^6 metric tons per year of ammonia, how much natural gas feed is necessary in metric tons per day and SCMH? Neglect the gas needed for the furnace. A year at the company consists of 350 days, 24 hours each day. SCMH = standard cubic meters/hr, where standard temperature and pressure are defined as T = 0°C and P = 1 atm.
9. What % of the original hydrocarbon feed is lost in the purge stream?

Part 2 - Energy Balance Questions: Let G = 100 mol/s unless stated otherwise

10. FEED:
    (a.) If the natural gas feed (G) starts at 25ºC and 1 atm, how much total heat (in kW) is needed to pre-heat the natural gas feed to 600ºC isobarically?
    (b.) If the liquid water feed (W) starts at 25ºC and 1 atm, how much total heat (in kW) is needed to pre-heat the water feed to vapor at 600ºC isobarically?
11. PRIMARY REFORMER: How much heat is needed for the primary reformer to have an exit temperature of 760ºC?
12. FURNACE FOR PRIMARY REFORMER: Additional natural gas is combusted with 25% excess air (both initially at 25ºC and 1 atm) in a furnace to provide heat for the reformer. The combustion exhaust gases exit the furnace at 900ºC. Assume only complete combustion reactions occur and assume 100% conversion of all hydrocarbons. Assume half of the heat from the furnace is transferred through the furnace walls into the reformer. For G = 100 mol/s, what flow rates of natural gas and air are needed for the furnace?
13. SECONDARY REFORMER: For the secondary reformer, air is pre-heated from 25ºC to 600ºC isobarically at 1 atm.
    (a.) How much heat is required?
    (b.) If the exhaust gases at 900ºC from question 5 are used to heat this air (in a heat exchanger with perfect efficiency), what is the final temperature of exhaust gases?

14. FINAL: In order for the ammonia plant to be profitable, the amount (mol/s) of ammonia produced MUST be greater than the total amount (mol/s) of natural gas used. It MUST also be at least 10% of the total amount (mol/s) of air used.
    (a.) What are the ratios of ammonia/natural gas and ammonia/air?
    (b.) Is the plant profitable?

Appendix A3. Sample Group Project Assignment for *Chemical Engineering Thermodynamics*

(Haber-Bosch process for ammonia synthesis Introduction and History, Process Description, and Process Flow Diagram sections are provided in Appendix A1.)

Your Assignment:

Analyze the provided plant design to determine the amount of ammonia product that can be produced under the conditions provided. You will utilize the material and energy balances developed in your Material and Energy Balances course, and modify them with the new knowledge you have developed in Chemical Engineering Thermodynamics. Our goal is to determine various operating conditions and whether the current setup of the plant will be profitable.

Project Goal:

The purpose of this project is to modify the basic assumptions we made in this plant from Material and Energy Balances and correct our calculations. You will compare how this plant operates under idealized conditions (ideal reactors, ideal gases, ideal separation units) with more realistic conditions. This is the first time we are continuing this project since Material and Energy Balances, and it will be expanded upon again in your future classes.

Process Design Features:

(1) Treat G = 100 mol/s and W = 268.5 mol/s

(2) The water is provided by a nearby lake and pumped in at 25ºC and 5 bar. Both the water and natural gas feed streams start at 25ºC and 5 bar, but are pre-heated to 400ºC then compressed to 35 bar. The fresh feed compressor operates at 85% efficiency.

(3) The primary reformer operates at 760ºC and 35 bar.

(4) All ethane, propane, and butane are consumed in the primary reformer.

(5) The methane reforming and WGS reactions are equilibrium limited. At reactor conditions, the gases can be treated as ideal.

(6) Pressurized air at 25ºC and 5 bar is pre-heated to 400ºC and then compressed to 35 bar before entering the secondary reformer. The air compressor operates at 85% efficiency.

(7) The secondary reformer operates at 1000ºC and 35 bar. The reaction goes to completion.

(8) Stream S goes through a heat exchanger and is cooled to 400ºC before entering the shift reactor.

(9) The shift reactor operates at 300ºC and 35 bar. The reaction goes to equilibrium as defined by the WGS equilibrium above in Feature #5.

(10) In Condenser #1, stream L is cooled to 150ºC, where all water is assumed to be removed into stream C.

(11) In the PSA, all CO and CO_2 are removed and leave in stream T.

(12) In streams B, RF, E, V, R, and P, the ratio of H_2:N_2 is 3:1. Note, CH_4 is still present.

(13) Stream B passes through a compressor where the pressure is increased from 35 bar to 175 bar. The efficiency of this “pre-recycle” compressor is 70%.

(14) At the mixing point, streams B and R mix and stream RF is then heated to 1000ºF before entering the isothermal ammonia reactor.

(15) The ammonia reactor operates at 1000ºF and 175 bar and goes to equilibrium.

(16) The ammonia reactor exhaust (stream E) passes through a turbine to recover work and decompress the gas stream to 7 bar. The ammonia turbine operates at 80% efficiency.

(17) The condenser cools the turbine exit stream to 0ºC where all ammonia is assumed to condense out of stream E and into stream N (the final product).

(18) Of all the vapors in stream V, 99% is recycled into stream R, while the remainder is purged in stream P.

(19) Finally, the vapors in stream R are compressed back to 175 bar before mixing with stream B. The recycle compressor operates at only 60% efficiency.

(20) VAPORS WILL NO LONGER BE TREATED AS IDEAL GASES UNLESS STATED OTHERWISE.

Project Equations:

Calculating residuals for gas mixtures:

Create averaged parameters for the entire flow instead of calculating residuals for individual components. Note: “pc” means pseudocritical and “pr” means pseudoreduced. Also, when in mixtures, ω for H_2 should always be taken as 0.

$$\omega_{mix} \equiv \sum_i y_i \omega_i \qquad T_{pc} \equiv \sum_i y_i T_{ci} \qquad P_{pc} \equiv \sum_i y_i P_{ci} \qquad T_{pr} \equiv \frac{T}{T_{pc}} \qquad P_{pc} \equiv \frac{P}{P_{pc}}$$

Primary Reformer & Shift Reactor Equilibrium Equations:

$$K_{R1,CH4} = \frac{p_{CO} p_{H2}^3}{p_{CH4} p_{H2O}} \qquad \log\left(K_{R1,CH4}\right) = \frac{-11{,}769}{T(K)} + 13.1927$$

$$K_{WGS} = \frac{p_{CO2} p_{H2}}{p_{CO} p_{H2O}} \qquad \log(K_{WGS}) = \frac{1197.8}{T(K)} - 1.6485$$

NH3 Synthesis Reactor Species Balances:

$$RF = 100B - 396\xi \qquad E = RF - 2\xi = 100B - 398\xi$$

$$y_{CH4}^E = \frac{100 y_{CH4}^B B}{E} \qquad y_{H2}^E = \frac{100 y_{H2}^B B - 300\xi}{E} \qquad y_{N2}^E = \frac{100 y_{N2}^B B - 100\xi}{E} \qquad y_{NH3}^E = \frac{2\xi}{E}$$

$$\log(K_{NH3}) = \frac{3629.3}{T(K)} - 8.9596 \qquad K_{NH3} = \frac{\left(\hat{f}_{NH3}/f_{NH3}^o\right)^2}{\left(\hat{f}_{N2}/f_{N2}^o\right)\left(\hat{f}_{H2}/f_{H2}^o\right)^3}$$

% Error and % Change:

$$\%\,Error = 100\% \left|\frac{estimate - actual}{actual}\right| \qquad \%\,Change = 100\% \left|\frac{new - old}{old}\right|$$

Henry's Law Dependence on Temperature:

$$\ln\left(\frac{H_2}{H_1}\right) = \frac{-E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Project Material Properties:

Most of the physical properties you need can be found in your textbook Appendix (Introduction to Chemical Engineering Thermodynamics, 9th ed. by Smith, Van Ness, Abbott, and Swihart). You will also need the properties below:

Henry's Law Constants for Water:

Species	**H at 25ºC (in bar)**	**E_a/R (K)**
Methane	39000	1600
CO	55500	1300
CO_2	1550	2400
H_2	70000	500
N_2	90000	1300

Henry's Law Constants for Ammonia:

Species	**H at 25ºC (in bar)**	**E_a/R (K)**
Methane	17800	-2000
H_2	15200	-1700
N_2	8900	-1600

*Note: in ammonia, these species will dissolve MORE as T increases

Antoine's Constants for Ammonia:

$$\ln P^{sat}/kPa = 15.3803 - \frac{2308.8}{T/°C + 247.885}$$

Heat Capacity for Liquid Ammonia:

$C_P/R = 9.72$

Process Question (to be completed in teams of 3-5 students):

1. FEED PRE-TREATMENT: Initially assume ideal gases.
    a. How much heat is necessary to heat both streams isobarically from 25ºC to 400ºC?
    b. How much work is required to compress the combined feed vapors from 5 bar to 35 bar? What is the corresponding final temperature of the combined streams?
    c. Using the pre-compression state and the final state of the combined feed, calculate the enthalpy residuals. Do not re-solve part b. What is the error of neglecting residuals?
2. PRIMARY REFORMER: How much heat is needed for the primary reformer to operate isobarically with the exhaust (stream F) at 760ºC? Treat gases as ideal.
3. AIR PRE-TREATMENT: Assume air is an ideal gas composed of only O_2 and N_2.
    a. How much heat is necessary to heat the air isobarically from 25ºC to 400ºC?

b. How much work is required to compress the air from 5 bar to 35 bar? What is the corresponding final temperature?

4. SECONDARY REFORMER: How much heat is necessary for the secondary reformer to operate with an exhaust temperature of 1000ºC? Assume ideal gases.
5. SHIFT REACTOR: Assume ideal gases.
   a. How much heat must be removed to cool stream S to 400ºC before the reactor?
   b. How much heat must be removed from the reactor if the exhaust is at 300ºC?
6. WATER CONDENSER: Assume ideal gases. Only water will condense in this step.
   a. How much heat must be removed to cool the streams to 150ºC?
   b. It was initially assumed that none of the components in stream D are lost in stream C, but this is not exactly true. Use the Henry's Law data provided to determine the mole fraction of all these components in stream C. Was our original assumption justified?
7. PRE-RECYCLE COMPRESSOR: Initially assume ideal gases.
   a. How much work is necessary to compress stream B to 175 bar?
   b. What is the corresponding final temperature after compression?
   c. Calculating the residuals for the initial and final state, how much error was introduced in the work calculation by assuming ideal gases? (Do not re-calculate a or b)
8. AMMONIA REACTOR: The ammonia reactor must operate at 1000ºF and 175 bar.
   a. How much heat is required to keep the MeOH reactor isothermal? Consider the vapors as ideal gases in this part alone.
   b. If the vapors in the reactor act as an ideal solution, but non-ideal gases, re-calculate the composition of the exhaust for this non-ideal system. Utilize the material balance equations provided. Do not iterate. Solve by any means necessary.
   c. If the original values are used, find the error in the flow rates of streams E & N.
9. AMMONIA TURBINE: After the ammonia reactor, the stream passes through a turbine to expand the mixture and reduce the pressure. Assume ideal gases.
   a. How much work is obtained from expanding stream E (initially at 1000ºF) from 175 bar to 7 bar?
   b. What is the final temperature of this stream after the turbine?
10. CONDENSER 2: Assume ideal gases. Only ammonia will condense in this step.
    a. How much heat must be removed to cool the streams to 0ºC?
    b. Using the Henry's Law constants for materials in liquid ammonia provided, what are the mole fractions of the other components? Was our original assumption of virtually pure ammonia in stream N justified?
11. RECYCLE COMPRESSION: The recycle stream must be pumped back up to 175 bar before being mixed with stream B and sent into the reactor. Assume ideal gases.
    a. How much work is required to compress stream R back to 175 bar?
    b. What is the final temperature after compression?
12. AMMONIA STORAGE: Liquid ammonia is typically held in storage tanks before being transported for sale or processing. A 90,000 gallon tank is evacuated before being filled with ammonia. Safety guidelines state that, at maximum, only 85% of the tanks by volume can be filled with liquid, leaving the remaining space as vapor ammonia.
    a. If the tanks are held at 25ºC, what pressure must the tanks be able to maintain internally?
    b. How long will it take to fill a tank to safety capacity (from being completely empty) given the basis used in Process Design Feature #1?

Appendix A4. Sample Group Project Assignment for *Chemical Reaction Engineering*

In this project we'll continue the analysis of the Haber-Bosch ammonia production process introduced in Material and Energy Balances and Chemical Engineering Thermodynamics. It's not necessary to have completed those projects in order to complete this project. Our emphasis in this class will be on the ammonia reactor.

You must complete this project in teams of 3-6. Submissions from teams of less than 3 or more than 6 will receive 0 points. A summary sheet is included on the Canvas page where this file was found, which you must include as a cover page on your completed project.

Review

The ammonia loop in Material and Energy Balances and Thermodynamics utilized a classic reactor-separator-recycle-purge (RSRP) loop as shown in Figure 1. The reactor was modeled as an equilibrium reactor and the separator "perfectly" removed all ammonia as product in stream N. A purge stream P allowed removal of inert gases.

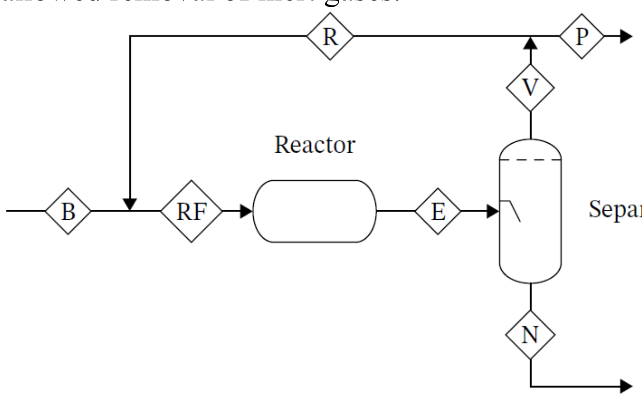


Figure 1: Reactor-separator-recycle-purge (RSRP) loop for ammonia synthesis. Stream B was the output from the reformer loop which produced H_2 and N_2 from steam and natural gas. Heat exchangers and recovery turbine not shown.

In this class we'll focus only on the reactor and its feed and effluent streams, RF and E. Previously this reactor was assumed to operate at equilibrium (i.e., an equilibrium reactor) but here we'll treat it as a packed-bed reactor. More specifically it is usually a series of packed bed reactors with feed preheat and interstage cooling. We'll build up to this complexity a little bit at a time, starting from a single reactor, then introducing feed preheat, and finally accounting for interstage cooling.

Temkin-Pyzhev Kinetics

Ammonia is produced from nitrogen and hydrogen according to the gas phase, non-elementary reaction

$$N_2 + 3H_2 \rightleftarrows 2NH_3$$

which is presumed to follow Temkin-Pyzhev kinetics as provided by Froment et al. [17] as described by the rate equation

$$r' = \frac{f}{\rho_{bed}}\left(k_1 \frac{p_{N_2} p_{H_2}^{1.5}}{p_{NH_3}} - k_2 \frac{p_{NH_3}}{p_{H_2}^{1.5}}\right) \quad (kmol\ kg_{cat}^{-1} h^{-1}) \tag{1}$$

where

$$k_1 = 1.79 \times 10^4 e^{-87.1/RT}$$

$$k_1 = 1.79 \times 10^4 e^{-87.1/RT}$$

$$f = 4.75$$

In these expressions p_i is the partial pressure of species i (in bar), and activation energies have units of kJ mol^{-1}. The bed contains 1/8" diameter catalyst particles packed to a bed density of 2200 kg$_{cat}$ m^{-3} and a void fraction ϕ = 0.35.

<u>Problem 1</u>

Consider the adiabatic, packed bed reactor shown in Figure 2. A gas stream 25% N_2, 65% H_2, 5% NH_3 and the balance CH_4 (an inert) enters the reactor at 275°C, 200 bar, and at a total molar flow rate of 5040 kmol h^{-1}. These conditions are approximately equivalent to the conditions calculated in Chemical Engineering Thermodynamics for stream RF.

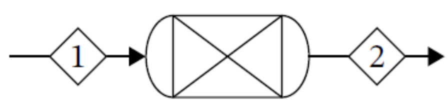


Figure 2: Process flow diagram (PFD) for Problem 1.

The reactor diameter is 1 m. Assuming pressure drop follows the KTA expression with $\mu = 1 \times 10^{-5}$ Pa s, determine the length of reactor required for the reaction to approach equilibrium (i.e., the length needed for compositions to mostly stop changing). For this and all remaining problems assume the heat capacities of each species are constant and equal to their values at 700K.

Create a 3-by-1 subplot figure with the molar flow rate profiles (in kmol h^{-1}) within the reactor of all species except CH_4 on the left, reactor temperature (in °C) in the center, and reactor pressure on the right. The x-axis of both plots should be reactor length L (in m). On the summary page, fill in the required stream table values. Also calculate the conversion of H_2 and the net production rate (in kmol h^{-1}) of NH_3.

Feed Preheat

Most industrially-relevant chemical reactions are exothermic and the energy given off by such reactions should be put to use rather than rejected to the environment. One option is to use the hot product stream to warm up a cool reactant stream in a process called feed preheat.

As shown in Figure 3(A) the fresh, cold feed is sent through a heat exchanger where it's heated by the hot reactor products. Importantly, the streams within the heat exchanger do not mix but only transfer energy. A description of the relevant governing equations for heat exchangers is provided in Appendix: Heat Exchangers.

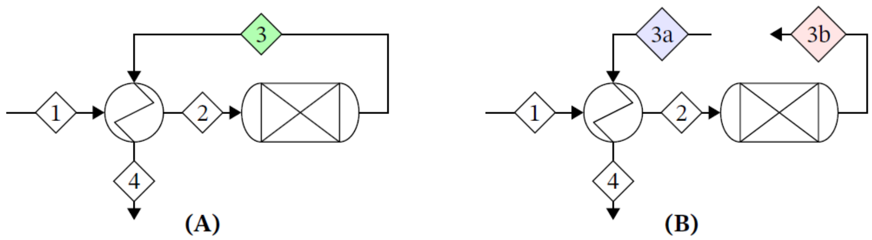


Figure 3: Reactor with feed pre-heat. (A) Feed stream 1 passes through a heat exchanger and is heated by reactant effluent stream 3. (B) An example of stream tearing use on stream 3, broken into 3a (the "guessed" stream) and 3b (the "checked") stream.

Such recycle behavior typically requires an iterative solution. The method to be used on this project is called stream tearing and proceeds as follows:

a. A suitable "tear stream" is identified. This must be part of the recycle loop and is usually selected for its computational convenience. In Figure 3(A) the tear stream is stream 3.

b. The stream is "torn" somewhere in its middle. In Figure 3(B) stream 3 has been torn into streams 3a and 3b.

c. One of the tear streams is called the "guessed" stream. The composition and properties of this stream are guessed so that computation of the recycle loop can begin. In Figure 3(B) stream 3a is the guessed stream such that streams 2 and 4 can be calculated, followed by stream 3b.

d. The other tear stream is called the "check" stream. Its purpose is to serve as a means of checking the accuracy of the guessed stream. In Figure 3(B) stream 3b is the check stream.

e. If the guessed stream is sufficiently similar to the checked stream then iteration halts. If the two are dissimilar then iteration continues, with the next guess being the checked value (i.e., 3a becomes equal to the calculated 3b, and the calculation repeats). This process is called successive substitution.

Problem 2

Assume stream 1 from Problem 1 is the same as stream 1 in Figure 3. The reactor now has a fixed length of 3m and the heat exchanger has an area of 500 m^2. Determine the composition of all streams using the tear stream approach described above. Assume there is no pressure drop across the heat exchanger.

Create a 3-by-1 subplot figure like the one in Problem 1. Create an additional plot in a new figure which contains the molar flow rates for N_2, H_2, and NH_3 in stream 3b at each step of the iteration (the x-axis should be iteration number). This plot is called a convergence plot and should serve to illustrate how the iterative process converges to stable numerical values for the flows in stream 3b.

On the summary page fill in the required stream table values, namely:

- A stream table containing the first three values of 3b and the last two values of 3b from your iteration process.
- A separate stream table for all streams in the process, assuming stream 3 is equal to the last value of stream 3b.

Interstage Cooling

There are several different layouts used by "real" ammonia plants for their reactors, most containing an implementation of interstage cooling. Interstage cooling reduces the temperature (and sometimes, changes the composition) of a reactor effluent stream before sending the so-modified stream into yet another reactor. The process often continues for three or more reactors.

One arrangement is shown in Figure 4 and is functionally identical to the arrangement provided in Araújo and Skogestad [18]. There are many important features to this process:

1. Stream 1 has the same composition and temperature as the inlet streams in the previous two problems (not stream RF).
2. The primary reactor feed (RF), initially at 50 °C, is preheated by H-101 before being split into four substreams: stream 2 is heated still further while streams 3, 4, and 5 remain at the same temperature.
3. Stream 2 contains 40% of stream 1, streams 3 and 4 each contain 25% of stream 1, and stream 5 contains the remaining 10% of stream 1.
4. A pressure regulator () automatically operates to ensure the pressure of stream 3 matches that of stream 10, and similarly for streams 4 and 8. This regulator is assumed to operate isothermally.

5. All reactor diameters are 1 m. Reactor lengths are 2, 3, and 4 m for R-101, R-102, and R-103.

6. The area of H-102 is 500 m^2. The area of H-101 is unknown.

7. Energy balances and solution techniques for heat exchangers and stream merge points are provided in the Appendix of this document.

8. All unit operations except reactors and the aforementioned pressure regulators are assumed to operate isobarically.

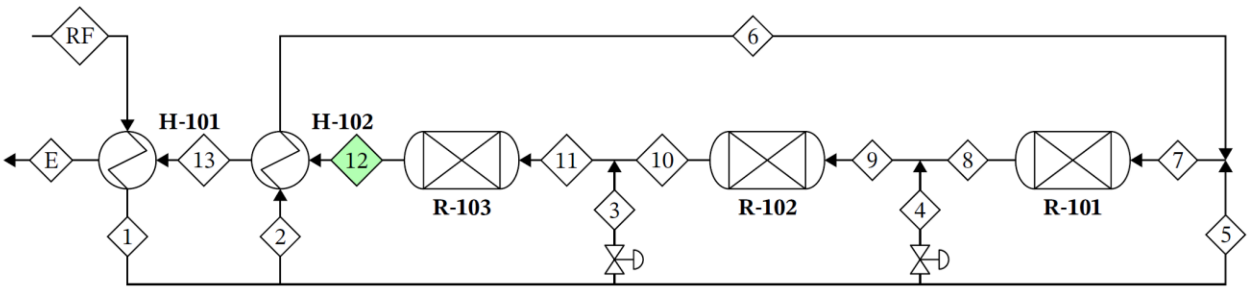


Figure 4: Reactors with interstage cooling and pre-heat. Note that stream 1 composition is given (same as in previous problems) but stream RF is unknown. Stream 12 is highlighted as the tear stream. Energy balances and solution approaches for stream merge points and heat exchangers are provided in the Appendix of this document.

<u>Problem 3</u>

Calculate the temperatures and compositions of all streams in Figure 4, subject to the features listed above. Use stream 12 as your tear stream. Create 2-by-1 subplot figures for each of the reactors, with molar flow rate profiles on the left, temperature profiles on the right, and a title indicating the relevant reactor. In a separate figure create a convergence plot for stream 12b as you did for stream 3b in Problem 2.

On the summary page fill in the required stream table values as well as the overall conversion of H_2, the net production rate (in kmol h^{-1}) of NH_3, and the area of H-101.

Appendix

Heat Exchangers

A heat exchanger is a unit which transfers energy (in the form of heat) between two streams. The streams do not mix but rather transfer energy across a mechanical barrier, typically a metal such as copper or stainless steel. One fluid is referred to as the tube-side fluid because it flows within a tube (or tubes), while the other fluid is referred to as the shell-side fluid because it flows over a tube (or tubes), as shown in Figure 5.

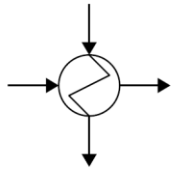


Figure 5: A basic heat exchanger. The tube-side fluid does not make physical contact with the shell-side fluid. Fluids need not be the same phase.

Each side must be specified as either the “hot” stream or the “cold” stream: the “hot” stream is the stream coming in at a high temperature and the “cold” stream is the stream coming in at a low temperature. For this project it doesn’t matter which side of the exchanger the streams are on.

The governing equations for a heat exchanger are three: two energy balances–one for the hot stream, one for the cold stream–and one empirical relationship describing the effectiveness of heat transfer. These three equations are

$$Q = \sum^{hot} n_i C_{P,i}(T_{h0} - T_h) \tag{2}$$

$$Q = -\sum^{cold} n_i C_{P,i}(T_{c0} - T_c) \tag{3}$$

$$Q = UA\Delta T_{lm} \tag{4}$$

where h and c subscripts refer to the hot and cold streams, Q is the energy transferred between the two streams, A is the surface area of the heat exchanger, and ΔT_{lm} is the log-mean temperature difference,

$$\Delta T_{lm} = \frac{\Delta T_2 - \Delta T_1}{\ln \frac{\Delta T_2}{\Delta T_1}}$$

where $\Delta T_1 = T_h - T_{c0}$ and $\Delta T_2 = T_{h0} - T_c$. This system of three equations can be used to solve for any three variables therein. Pressure drop across heat exchangers is assumed (somewhat questionably) to be negligible.

It’s often difficult to estimate Q a priori which makes it difficult to solve the three equations given above. Instead, Q can be eliminated to reduce the system to two equations and two unknowns as

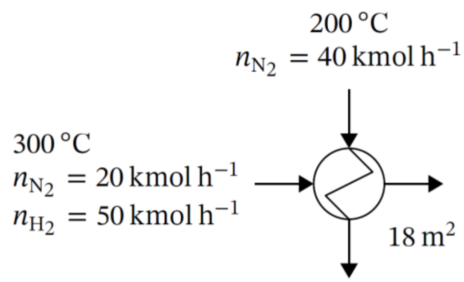
$$UA\Delta T_{lm} = \sum^{hot} n_i C_{P,i}(T_{h0} - T_h) \tag{5}$$

$$UA\Delta T_{lm} = -\sum^{cold} n_i C_{P,i}(T_{c0} - T_c) \tag{6}$$

These are usually the two equations used to solve for unknowns in heat exchanger problems.

Example: Heat Exchanger Calculation

Estimate the outlet stream temperatures for the following heat exchanger:



All streams are gas-phase. Heat capacities for N_2 and H_2 are assumed constant and equal to 31 J mol^{-1} °C^{-1} and 29 J mol^{-1} °C^{-1}. Equations (5) and (6) reduce to

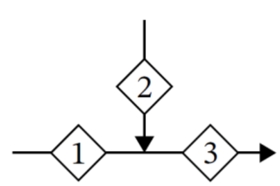
$$30 \cdot 18\Delta T_{lm} = (20 \cdot 31 + 50 \cdot 29)(300 - T_h)\frac{1000}{3600}$$

$$30 \cdot 18\Delta T_{lm} = (20 \cdot 31 + 50 \cdot 29)(300 - T_h)\frac{1000}{3600}$$

where $\Delta T_1 = T_h - 200$ and $\Delta T_2 = 300 - T_c$. Solving yields T_h = 258.9 °C (for the N_2, H_2 stream) and T_c = 268.6 °C (for the pure N_2 stream).

Stream Merging

Consider the following stream merger:



The molar flow rates of stream 3 are the sum of the molar flow rates of streams 1 and 2, and the pressures of all three streams are equal. The temperature of stream 3 can be estimated by an enthalpy balance.

$$\sum^{inlets} n_i H_i = \sum^{outlets} n_i H_i$$

$$\sum n_{i,1} H_{i,1} + \sum n_{i,2} H_{i,2} = \sum n_{i,3} H_{i,3}$$

Taking stream 1 as the reference state implies $H_{i,1} = 0$. Assuming any individual species enters and leaves the merger without changing phase, each remaining enthalpy can be estimated as $H_i = C_{P,i}\,(T_i - T_1)$. Substituting and rearranging yields

$$T_3 = \frac{\sum n_{i,2} C_{P,i}}{\sum n_{i,3} C_{P,i}} (T_2 - T_1) + T_1.$$

Appendix A5. Sample Group Project Assignment for *Chemical Process Dynamics and Control*

(Haber-Bosch process for ammonia synthesis Introduction and History, Process Description, and Process Flow Diagram sections are provided in Appendix A1.)

Your Assignment:

You desire to control the temperature of the ammonia reactor, as shown in the overall process flow diagram. You are provided either the process transfer functions or relative figures/plots. Analyze the process response, the open loop response, and the closed loop response. Tune the relevant controllers and plot the controlled response.

Project Goal:

The purpose of this project is to incorporate all the concepts learned in your prior chemical engineering courses and design a controller. You will apply control concepts learned in this course to analyze the dynamics of the reactor and develop optimum control parameters for them. This is the penultimate time we are considering this project since Material and Energy Balances, and by the end of this year, we will have completed a full analysis of the Haber-Bosch process.

Process Design Features:

Production of Ammonia from Natural Gas: Ammonia Reactor Analysis

In the second half of the process (lower half of process flow diagram above), feed gas (N_2 & H_2 in stoichiometric ratio, with trace CH_4) is reacted at extremely high pressure and temperature to produce ammonia:

Ammonia Synthesis Reaction: $N_2 + 3H_2 \leftrightarrow 2NH_3$

The reactor operates near 1000ºF at pressures over 2500 psia.

A linearized process model for the temperature response to changing coolant flow rate (both as deviation variables) is determined to be:

$$\frac{T(s)}{F_c(s)} = G_p(s) = \frac{-35.77(2.07s+1)}{26.27s^3 + 36.31s^2 + 10.14s + 1}\frac{ºR}{ft^3/min}$$

A linearized process model for the temperature response to changing inlet temperature (both in deviation variables) is determined to be:

$$\frac{T(s)}{T_{in}(s)} = G_D(s) = \frac{1.31(2.07s+1)(0.976s+1)}{26.27s^3 + 36.31s^2 + 10.14s + 1}\ \frac{ºR}{ºR}$$

The thermocouple has transfer function (with time constant in units of minutes):

$$G_T(s) = \frac{1}{0.3s+1}\frac{\%TO}{ºC}$$

The valve actuator manipulating fluid flow has transfer function:

$$|G_V(s)| = \frac{1}{0.05s+1}\frac{L/min}{\%\,CO}$$

Process Question (to be completed in teams of 3-5 students):

Part 1: Tuning Based on Ultimate Gain

Using Matlab and/or Simulink:

1.) Determine the process response (in ºC) to a 0.5 L/min increase in coolant flow. Provide the response curve.
2.) Determine the disturbance response (in ºC) to a 10ºC increase in inlet temperature. Provide the response curve.
3.) The temperature is critical. If it drops significantly, reaction equilibrium is reduced to near zero. Is the desired valve fail-open (air-to-close) or fail-closed (air-to-open)? What controller action is necessary? Reverse or direct? Explain.
4.) Show the closed loop process diagram with the controller.
5.) Determine the open-loop system response (including actuator and sensor), in ºC, to a step increase of 0.5 in controller signal (AKA % CO). Show the response curve.
6.) Provide the Root Locus diagram for this system. Take special note if you want the diagram for positive or negative Kc-values.
7.) Calculate the ultimate gain, Kcu, and the ultimate period, Pu for the open-loop process.
8.) Calculate the Ziegler-Nichols (ZN) parameters for both PI- and PID-control.
9.) Determine the system response to a step set point increase of 10ºC for both sets of ZN parameters from #8. Plot on the same axes. Provide a legend. Compare the two plots. Is one controller clearly better than the other? Why or why not?

*** Note: when using Derivative-Control, assume a filter is used, with $\alpha = 0.1$.

Part 2: Tuning from FOPDT Parameters for Setpoint Changes

Using Matlab and/or Simulink:

1.) Determine the FOPDT parameters for the process.
2.) Determine the FOPDT parameters for the open-loop system response.
3.) Determine the FOPDT parameters for the disturbance.
4.) For tuning purposes, which set of FOPDT parameters should be used? Why?
5.) Calculate the Ziegler-Nichols (ZN) and Cohen-Coon (CC) parameters for both PI- and PID-control for set-point changes. Tune based off of the FOPDT parameters.
6.) Plot the closed-loop feedback response to a 10ºC increase in the set point using all four sets of control parameters from #5. Plot on the same axes. Provide a legend.

7.) Calculate the Integral of Absolute Error (IAE) and Integral of Time-Weighted Absolute Error (ITAE) parameters for both PI- and PID-control for set-point changes.
8.) Repeat #6 using the parameters from #7.
9.) Comparing all set-point tuning parameters determined in Parts 1 and 2 (both ZN, CC, IAE, and ITAE) for PI- and PID-control, which set would you choose? Compare and contrast the responses. Note: there is not necessarily a single correct answer.

*** Note: when using Derivative-Control, assume a filter is used, with $\alpha = 0.1$.

Part 3: Tuning from FOPDT Parameters for Disturbance Changes

1.) Plot the closed-loop feedback response to a 10ºC increase in the inlet temperature using the tuning settings found in Part 1 #8. Plot on the same axes. Provide a legend.
2.) Plot the closed-loop feedback response to a 10ºC increase in the inlet temperature using the tuning settings found in Part 2 #5. Plot on the same axes. Provide a legend.
3.) Calculate the Integral of Absolute Error (IAE), Integral of Square Error (ISE), and Integral of Time-Weighted Absolute Error (ITAE) parameters for both PI- and PID-control for disturbance changes.
4.) Plot the closed-loop feedback response to a 10ºC increase in the inlet temperature using all six sets of control parameters from #3. You can plot all six on one graph with proper labels. Alternatively, if the plot looks too cluttered, you can use 3 sets of graphs PI- vs PID- for each tuning set.
5.) Comparing all responses to disturbances (#1, #2, #4) for PI- and PID-Control, which set would you choose? Compare and contrast the responses. Note: there is not necessarily a single correct answer. Is one controller (PI vs PID) clearly better than the other, regardless of tuning method? Why or why not?

*** Note: when using Derivative-Control, assume a filter is used, with $\alpha = 0.1$.

Appendix A6. Sample Group Project Assignment for *Separation Processes*

(Haber-Bosch process for ammonia synthesis Introduction and History, Process Description, and Process Flow Diagram sections are provided in Appendix A1.)

<u>Your Assignment:</u>

Analyze the provided plant design to determine the extent of separation achievable in both condensers under the conditions provided. You will use your knowledge from this Separation Processes course to determine the best way to separate and purify desired chemical components.

<u>Project Goal:</u>

The purpose of this project is to modify the basic assumptions and calculations we made in Material and Energy Balances and Thermodynamics to design the separation units in the Haber-Bosch process. You will compare how this plant operates when separation is not perfect, and generally inefficient. Along with Chemical Process Dynamics and Controls, this will be the penultimate time you are exposed to this project - having now seen it from effectively every angle in terms of chemical engineering.

<u>Process Specifications:</u>

The shift reactor exit stream L is at 300°C and 35 bar with a total molar flow rate of 681 mol/s = 2451.6 kmol/hr and the following composition:

Species	Stream L mole fraction
CH_4	0.00175
CO_2	0.09127
CO	0.06469
H_2O	0.23328
H_2	0.45676
N_2	0.15225

The ammonia reactor exit stream E is at 1000°F and 175 bar with a total molar flow rate of 1180.4 mol/s = 4249.4 kmol/hr and the following composition:

Species	Stream E mole fraction
CH_4	0.10103
H_2	0.54520
N_2	0.18173
NH_3	0.17204

Energy Considerations:

Energy integration is of key importance in modern ammonia synthesis plants. High power compressors and pumps are necessary to achieve the necessary high pressures in the reactor. Work can be recaptured through turbines and expanders where the streams are decompressed. Heating/cooling utilities and heat exchangers are necessary to pre-heat the reactor feed and subsequently cool its exhaust. And the condensers (depending on the types of columns) could incorporate reboilers, condensers, and more heat exchangers. In this project, you will use Aspen to determine the energy requirements of the separation units.

Process Question (to be completed in teams of 3-5 students):

Part 1: Choosing a Thermodynamic Model

1.) Choose a thermodynamic model that you will use for each of the separators. EXPLAIN/JUSTIFY YOUR CHOICE AS TO WHY THAT IS LIKELY (ONE OF) THE BEST MODEL(S) TO USE. It is unlikely you will be using anything exotic, and also unlikely you'll need to change between separators, but if you do, explain.

Part 2: Modeling Condenser 1 (to remove as much water as possible)

In Material and Energy Balances, you used material balance and equilibrium relationships to find that the total molar flow rate of Stream L was 681 mol/s = 2451.6 kmol/hr with mole fractions given in the Process Specifications on page 5. In Thermodynamics, you assumed Condenser 1 condensed 100% of the water to liquid, and calculated a required heat duty of approximately -9000 kW. You also used Henry's law to determine that only a minimal amount of N_2 or H_2 was removed in the condensed water stream. Now, re-evaluate those assumptions by modeling in Aspen:

2A.) Model Condenser 1 using flash condensation at 35 bar and 150ºC. Report pressure, temperature, heat duty, molar flow rates of all components in streams L, C, and D, and mole fractions of all components in streams L, C, and D. Was the assumption that all the water vapor condensed to liquid an accurate assumption? What percentage of the water in stream L is removed in stream C under these conditions? What percentages of the H_2 and N_2 in stream L is removed in stream C under these conditions? Is the 1:3 ratio of N_2:H_2 significantly altered under these conditions?

2B.) Vary the flash condensation conditions (temperature and/or pressure) with the goal of condensing as much water as possible. (Use care to select reasonable conditions. Aspen calculates vapor-liquid equilibrium, but Aspen will not necessarily warn you if you enter conditions where water would be a solid.) <u>For 3 conditions</u>, report pressure, temperature, heat duty, molar flow rates of all components in streams L, C, and D, and mole fractions of all components in streams L, C, and D. What percentage of the water in stream L is removed in stream C under these conditions? What percentages of the H_2 and N_2 in stream L is removed in stream C under these conditions? Is the 1:3 ratio of N_2:H_2 significantly altered under these conditions?

2C.) Which of these conditions would you select for your final process, and why? Be sure to consider and discuss any trade-offs between water removal, N_2 or H_2 losses, and expected energy operating costs (pressure and/or heat duty).

Part 3: Modeling Condenser 2 (to remove ammonia product stream)

In Material and Energy Balances, you used material balance and equilibrium relationships to find that the total molar flow rate of Stream E was 1180.4 mol/s = 4249.4 kmol/hr with mole fractions given in the Process Specifications on page 6. In Thermodynamics, you calculated that approximately -14,000 kW of work was recovered by a turbine that expanded the reactor effluent from 175 bar to 7 bar. You also assumed Condenser 2 condensed 100% of the ammonia to liquid, and calculated a required heat duty of approximately -11,500 kW. You also used Henry's law to determine that only a minimal amount of N_2 or H_2 was removed in the condensed water stream. Now, re-evaluate those assumptions by modeling in Aspen:

3A.) Model a turbine with 80% mechanical efficiency that drops the ammonia reactor effluent pressure to 7 bar. Model Condenser 2 using flash condensation at 7 bar and 0°C. Report the net work recovered by the turbine and heat duty required for Condenser 2. Report for all streams (E1 before turbine, E2 after turbine, V, and N): pressure, temperature, molar flow rates of all components, and mole fractions of all components. Was the assumption that all the ammonia vapor condensed to liquid an accurate assumption? What percentage of ammonia is recovered in stream N under these conditions?

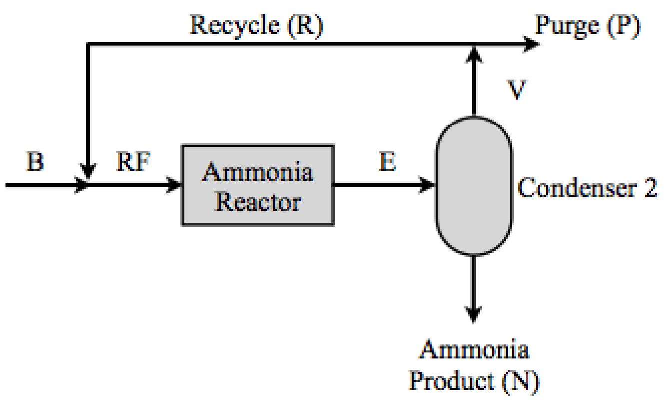
3B.) Vary the turbine and/or flash condensation conditions (temperature and/or pressure) with the goal of condensing as much ammonia as possible. (Use care to select reasonable conditions. Aspen calculates vapor-liquid equilibrium, but Aspen will not necessarily warn you if you enter conditions where ammonia would be a solid.) For 3 conditions, report net work recovered by the turbine, heat duty for condenser, and all stream pressures, temperatures, molar flow rates of all components, and mole fractions of all components. What percentage of ammonia is recovered in stream N under these conditions? What percentages of the H_2 and N_2 are lost in stream N under these conditions? Is the 1:3 ratio of N_2:H_2 in the recycle significantly altered under these conditions?

3C.) Which of these conditions would you select for your final process, and why? Be sure to consider and discuss any trade-offs between ammonia recovery, N_2 or H_2 losses, effect on reactor due to resulting recycle stream composition, and expected energy operating costs (pressure and/or heat duty and/or work).

Appendix A7. Sample Homework Assignments for *Chemical Plant and Process Design I*

Individual Homework Assignment 1: Modeling the Ammonia Synthesis Loop in Aspen Plus

Last quarter in Separation Processes and Chemical Process Dynamics and Controls, you analyzed the Haber-Bosch process for ammonia synthesis. For this homework assignment, you will focus on modeling the ammonia synthesis loop in Aspen Plus:



Upstream of this ammonia Reactor-Separator-Recycle-Purge loop, the primary and secondary reformers produce hydrogen, CO, and CO_2 via reforming and water-gas shift reactions. Nitrogen is introduced via air in the secondary reformer. Pressure-swing absorption is used to remove the CO and CO_2, leaving the ammonia synthesis reactants H_2 and N_2 in stream B at a stoichiometric 3:1 molar ratio.

The specifications for this process are as follows:

- Use the PSRK property method in Aspen.
- All streams (B, RF, E, N, V, P, and R) are at P = 175 bar. *(The compressors and turbines have been removed from the process here to simplify it for this homework assignment.)*
- Stream B has a total molar flow rate of 416 mol/s = 1497.6 kmol/hr and the following composition: 0.3% CH_4, 74.8% H_2, and 24.9% N_2 (in mole %). Stream B is at P = 175 bar and T = 490^{o}C.
- The ammonia synthesis reaction $N_2 + 3H_2 \leftrightarrow 2NH_3$ reaches equilibrium in the ammonia synthesis reactor. The reactor is operated at T = 540^{o}C and P = 175 bar.
- The condenser is a flash condensation operated at P = 175 bar and T = -65^{o}C.

Recall from Material and Energy Balances, the reactor can be analyzed using single-pass conversion:

$$single\ pass\ conversion = \frac{moles\ H_2\ entering\ reactor\ in\ RF - moles\ H_2\ exiting\ reactor\ in\ E}{moles\ H_2\ entering\ reactor\ in\ RF}$$

and the overall process with recycle can be analyzed using overall conversion:

$$overall\ conversion = \frac{moles\ H_2\ entering\ process\ in\ B - moles\ H_2\ exiting\ reactor\ in\ P\ and\ N}{moles\ H_2\ entering\ process\ in\ B}$$

1.) First, model the ammonia synthesis reactor and condenser in Aspen Plus as described above **WITHOUT the recycle loop**.

- **a.)** What reactor block did you select and why? *(Aspen help menu or either of the Aspen textbooks on Canvas should be helpful with this selection.)*
- **b.)** Include a screenshot of your main flowsheet.
- **c.)** Include a screenshot of your stream results T, P, molar flow rate, and mole fractions for all streams. Make sure your stream names are properly labeled to allow for proper grading.
- **d.)** Calculate the percent conversion of hydrogen.

2.) Use a **sensitivity analysis** to evaluate the flash condensation operating temperature. Vary the flash temperature from -77^oC (just above the freezing point of pure ammonia) to 0^oC with 20 points.

- **a.)** Include a plot of ammonia mole fraction in stream N, ammonia mole fraction in stream V, ammonia molar flow rate in stream N, and ammonia molar flow rate in stream V as a function of flash temperature.
- **b.)** Discuss the results. How does the condensation temperature affect the purity of your final ammonia product? How does the condensation temperature affect the recovery of your ammonia product?

3.) Now, model the ammonia synthesis reactor and condenser as described above **WITH the recycle loop**. Use the provided process specifications including a condenser temperature of -65^oC. **Recycle 50% of stream V back to the reactor.** *(You can avoid errors by first right clicking and deactivating or deleting your sensitivity analysis before running the process with the recycle loop.)*

- **a.)** Include a screenshot of your main flowsheet.
- **b.)** Include a screenshot of your stream results T, P, molar flow rate, and mole fractions for all streams. Make sure your stream names are properly labeled to allow for proper grading.
- **c.)** Calculate the single-pass percent conversion of hydrogen and overall percent conversion of hydrogen.
- **d.)** Discuss the results. How does the single-pass conversion compare to the process without recycle? How does the single-pass conversion compare to the overall conversion?

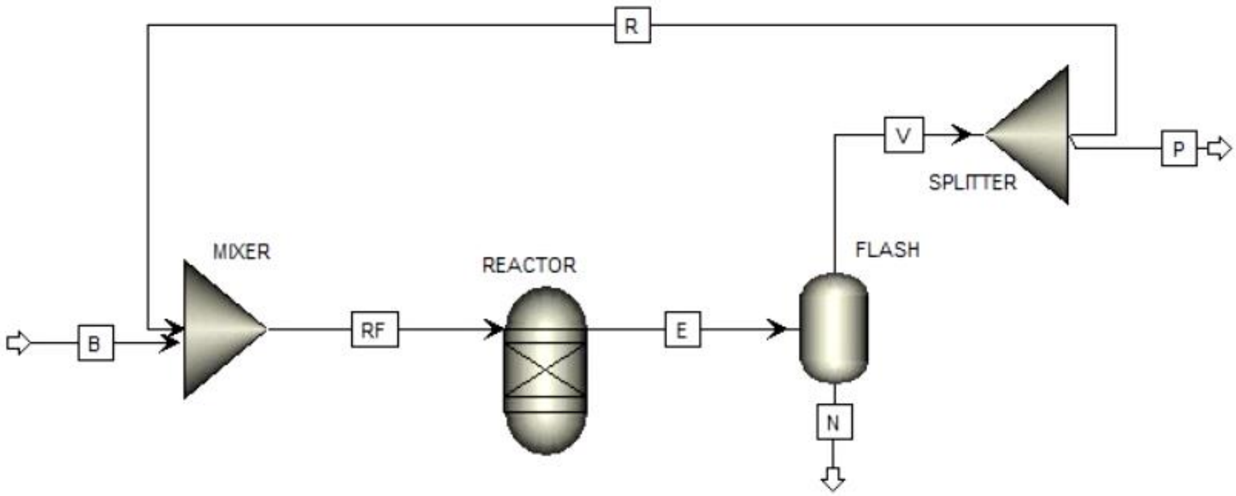
4.) Use the **Aspen calculator and design specs** to determine the percentage of stream V that should be purged to achieve an overall hydrogen conversion of 55%. (Recommendation: to avoid Aspen errors, when setting purge fraction as manipulated variable, don't set the purge fraction limit lower than 0.10).

- **a.)** Report the percent of stream V that should be purged to achieve 55% overall conversion.

*(**Just for fun**– you can also vary the reactor P and T and evaluate the effect on the equilibrium ammonia conversion. Why is the process operated at 175 bar?)*

Individual Homework Assignment 2: Pressure Vessel Design – Sizing the Condenser and Determining the Wall Thickness

For your project last quarter in Separation Processes and Chemical Process Dynamics and Controls, you analyzed the Haber-Bosch process for ammonia synthesis. For Homework 1, you modeled the ammonia synthesis reactor-separator-recycle-purge loop with flash condensation. The Aspen Plus flowsheet from Homework 1 Question 4 resulting in 55% overall conversion is shown below.



The stream results from the Aspen modeling for the same problem are shown below.

	Units	**N**	**V**
Phase		Liquid Phase	Vapor Phase
Temperature	C	-65	-65
Pressure	bar	175	175
Molar Density	kmol/m^3	33.2	8.9
Mass Density	kg/m^3	564.2	76.1
Average MW		17.00	8.58
Mole Flows	kmol/hr	408.1	3271.4
METHANE	kmol/hr	0.04	21.4
HYDROGEN	kmol/hr	1.1	2430.2
NITROGEN	kmol/hr	0.3	807.9
AMMONIA	kmol/hr	406.6	11.9
Mass Flows	kg/hr	6936.6	28076.9
METHANE	kg/hr	0.6	343.7
HYDROGEN	kg/hr	2.2	4899.0
NITROGEN	kg/hr	8.8	22631.9
AMMONIA	kg/hr	6925.0	202.3
Volume Flow	m^3/hr	12.3	368.8

BE VERY CAREFUL WITH YOUR UNITS.

1.) Based on the information above, calculate the required vertical **flash drum height and diameter** (**in meters, to 3 significant figures**) for the ammonia condenser.

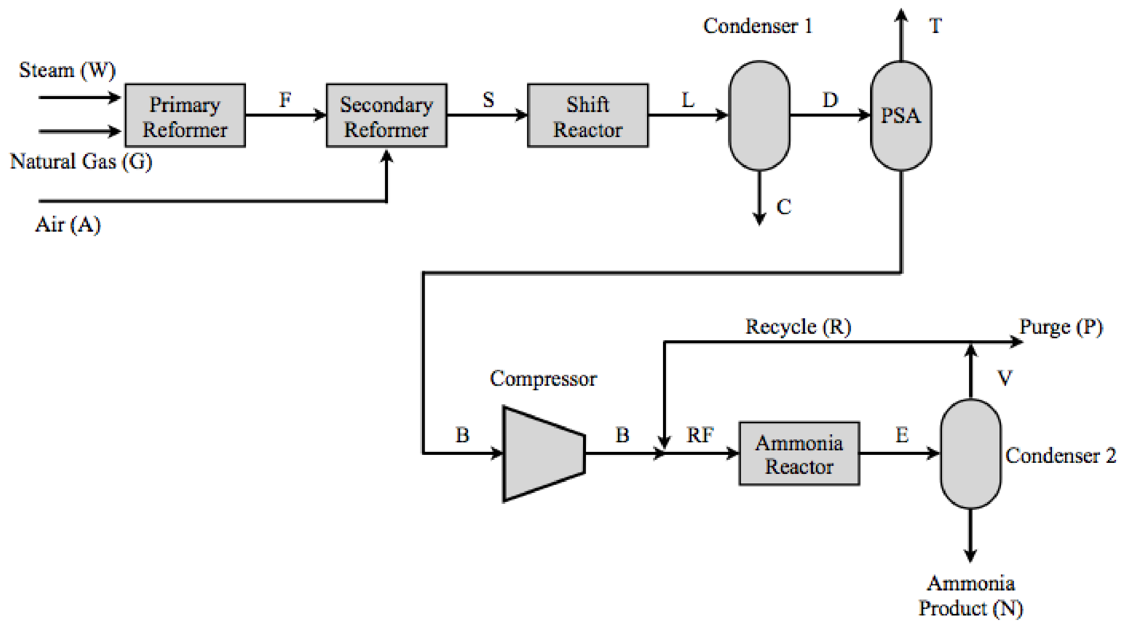
2.) Calculate the minimum wall thickness for the ammonia condenser. Initially, take the flash drum design pressure to be 10% higher than the normal working pressure of **175 bar** that you modeled in Homework 1. **Estimate the minimum wall thickness of both the cylindrical section and the ellipsoidal heads (in mm).** Design for plain carbon steel A285 (we can re-evaluate this choice of materials after we cover material selection next quarter). Assume a welded joint efficiency of 0.9.

3.) In practice, ammonia condensers are rarely operated above 10 bar. While the reactor must be operated at high pressure to drive reaction equilibrium towards the ammonia product, the reactor effluent is typically expanded in a turbine to drop the pressure and recover work. Take the ammonia condenser design pressure to instead be 10% higher than a normal working pressure of **7 bar**. **Estimate the minimum wall thickness of both the cylindrical section and the ellipsoidal heads (in mm**). Design for plain carbon steel A285. Assume a welded joint efficiency of 0.9.

4.) What is one advantage of decreasing the pressure between the ammonia reactor and the ammonia condenser? What is one disadvantage of decreasing the pressure before the condenser?

Individual Homework Assignment 3: Engineering Economics

Last quarter in Separation Processes and Chemical Process Dynamics and Controls, as well as on Homework 1 and Homework 2, you analyzed the Haber-Bosch process for ammonia synthesis:



Question 1)

Modeling the process gives the following flow rates:

- 100 mol/s natural gas is fed to the reforming reactor in stream G.
- 268.5 mol/s water is fed to the reforming reactor (after vaporizing to steam) in stream W.
- 203 mol/s ammonia is produced from the process in stream N.

Assume the following bulk chemical market price and industrial natural gas and water costs:

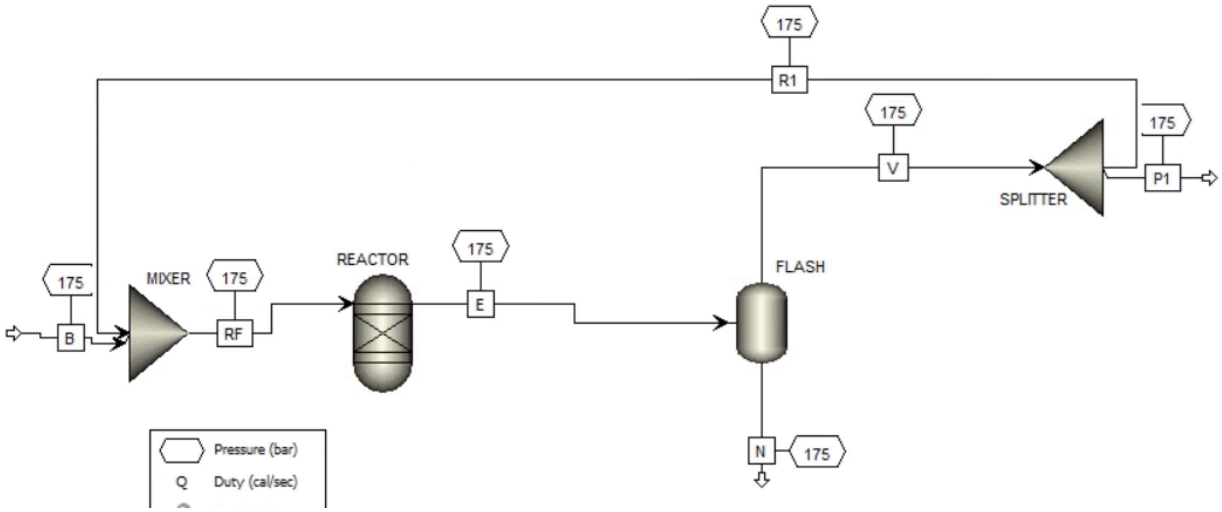
- \$503 per metric ton of ammonia.
- \$4.3 per thousand cubic feet of natural gas. Note: this price came from EIA (US Energy Information Administration) which reports natural gas volumes at a pressure of 14.73 psia and a temperature of 60ºF.
- \$3.38 per kGal (thousand US gallons) of water.

Determine the **gross margin (in \$/yr)** for the above process given the flow rates and prices above. Assume Sinnott and Towler's rule-of-thumb of 333 days/year or 8000 hours/year of operation for a continuous plant [19]. Show all your work for credit.

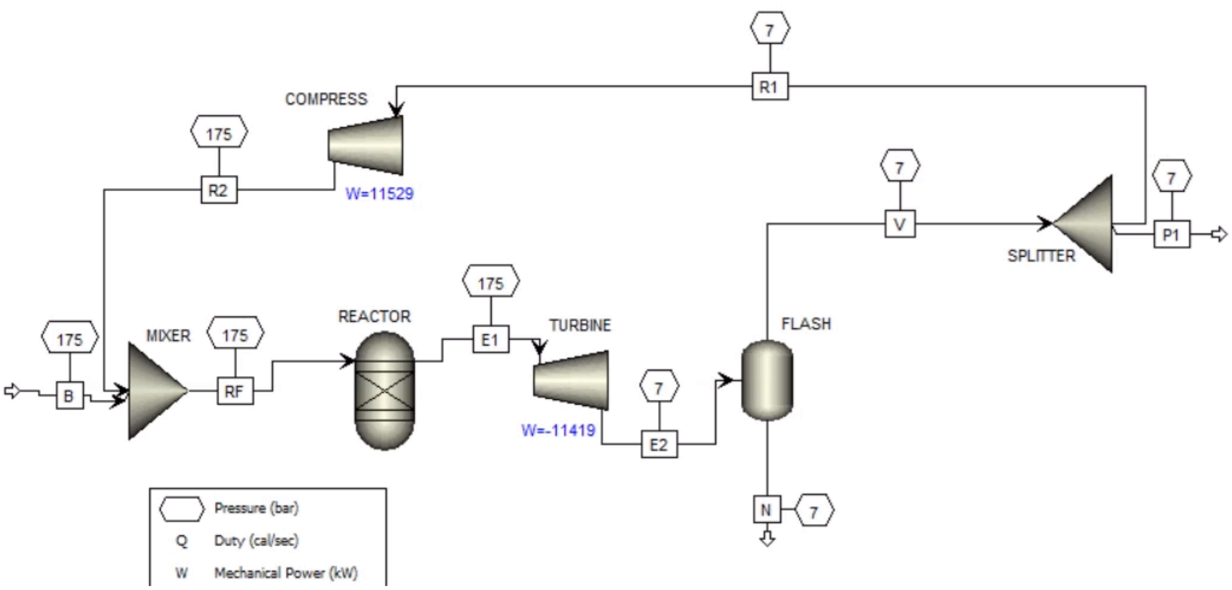
Question 2)

For Homework 2 (solutions posted on Canvas), you performed the sizing calculations for the ammonia condenser. You calculated the flash drum height and diameter as well as the pressure vessel wall thickness for two different process designs.

Design 1: operate the entire ammonia synthesis reactor-separator-recycle-purge loop at the constant reactor pressure of 175 bar, as shown below:



Design 2: expand the reactor product through a turbine (expander) to drop the pressure to 7 bar and recover work (W = -11,419 kW). Operate the ammonia condenser at 7 bar. Compress recycled vapor back to the reactor pressure of 175 bar, which requires work (W = 11,529 kW). This design is shown below.



a.) For Design 1 (condenser operated at 175 bar), use a flash drum height = 4 m, diameter = 1 m, and wall thickness = 141 mm. Estimate the **purchased equipment cost** and the **ISBL cost** given the following assumptions:

- Assume a vertical pressure vessel of plain carbon steel (we can re-evaluate this choice of materials after we cover material selection next quarter).
- Use the following from your Sinnott and Towler [19] course textbook: cost correlations from Table 6.6, vertical vessel mass from equation in example 6.2, carbon steel density from Table 7.2, and fluids processing plant factors for factorial method from Table 6.4.
- Assume the plant is to be built on the US Gulf Coast.
- Estimate the cost today using the 2022 annual CE cost index of 816 as a best-estimate for current cost index.

b.) Repeat the calculations for **purchased equipment cost** and the **ISBL cost** for Design 2 (condenser operated at 7 bar) with a wall thickness = 5 mm.

c.) Calculate the **annualized capital cost ACC** for both Design 1 and Design 2 if the project is financed with 15% interest and has an expected 10 year life of the plant.

d.) Calculate the annual compression costs for Design 2, assuming costs can be calculated from the net work W = -11,419 kW + 11,529 kW = 110 kW. Assume 8000 hours/year of operation for a continuous plant. Assume an electricity cost of $0.06/kWh.

e.) Comparing the ACC for Design 1 to the ACC and additional operating costs of Design 2, which design do you recommend and why?