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Incorporation of Sustainability Education into the Ammonia Synthesis Process Design of the Chemical Engineering Senior Design Course

Dr. Jia Li, California State Polytechnic University, Pomona

EDUCATION • Ph.D., Chemical Engineering, Wayne State University (GPA 3.98/4.0), 01/2007. Dissertation: Integrated Product and Process Research: A System Approach to Multiscale Complex Systems. • M.S., Chemical Engineering, Wayne State University (GPA 3.96/4.0), 2003. • M.S., Automation (chemical process control), Tsinghua University, Beijing, China, 2002. • B.S., Automation (chemical process control), Tsinghua University, Beijing, China, 1999.

WORKING EXPERIENCE Assistant Professor, Department of Chemical and Materials Engineering, Cal Poly Pomona, 2016 – present. • Teach Process Design and Process Control for senior students.

Process/Project Engineer, Wahlco Inc, Santa Ana, CA, 2014-2016. • Lead Urea to Ammonia process development. • Responsible for marketing research review. • Conduct internal and customer factory acceptance test. • Design process control system with PLC/DCS implementation.

Project Manager/Senior Engineer, ClearWaterBay Technology Inc. Pomona, CA, 2007-2014. • Managed a Large-scale Refinery Energy Optimization Project, 2012-2014. • Major project in process design: 30+ units and 2 utility systems, with both existing unit retrofit and new unit design. • Responsible for project management and most technical work. • 9-month on-site work with hand-on experiences. • Accepted ideas give ˜20 million US$ saving per year, which have been implemented into the engineering design. • Managed a Bio-ethanol Process Development Project, 2011-2012. • Conducted technical survey for conversion processes of cellulosic biomass to ethanol. • Identified pros and cons of different routes. • Performed integrated process simulation/modeling for production of ethanol from corn stover with acid pretreatment.

Technical Department Manager, ClearWaterBay (Beijing) Technology Inc., Beijing, China, 2011-2014. • Established CWB Beijing Company by interviewing engineers and building up sales group. • Supported sale work for various professional software and techniques.

Graduate Research Assistant, Wayne State University, Detroit, MI, 2002-2006. Summer Intern, Ford Motor Company, Advanced Manufacture Technology Developing Center (AMTD), Dearborn, MI, May-August, 2003. Process Engineer, Tsingda Smartech Co. Ltd., Beijing, China, 2002.

PROFESSIONAL SERVICE & HONORS • Session Chair, Modular Design and Process Intensification, the 9th International Conference on Foundations of Computer-Aided Process Design (FOCAPD), July 14-18, 2019, Copper Mountain, Colorado, USA. • Co-chair for 2018 AIChE Annual Meeting - Conceptual Process Design in Refining, Petrochemicals and Gas Processing. • Invited to 2017 SAChE (Safety and Chemical Engineering Education) Faculty Workshop in Richmond, CA, Aug. 2017. • Invited Speaker for 2017 WanHua Reactor Design Seminar in YanTai, ShanDong, China, June 2017. • DOE Qualified Steam System Specialist, US Department of Energy, 2009. • Member, American Institute of Chemical Engineers (AIChE), 2004-2008. • Presenter (four times), AIChE National Meeting, 2004, 2005 and 2006. • Paper Reviewer, Chemical Engineering & Processing and Computers & Chemical Engineering. • Vice Chair, Fourth Graduate Research Symposium, Wayne State Univ., Detroit, MI, 2004. • Lab Manager, Lab. for Multiscale Complex Sys. Sci. & Eng., Wayne State Univ., 2005-2007. • Summer 2006 Dissertation Fellowship, Wayne State Univ., 2006. • Albort Travel Award, Wayne State Univ., 2005. • Best Poster Award, Fifth Graduate Research Symposium, Wayne State Univ., 2005. • Best Presenter Award, Fourth Graduate Research Symposium, Wayne State Univ., 2004. • Second Prize of Tsinghua Scholarship, Tsinghua University, China, 1999. • Second Prize of Tsinghua Scholarship, Tsinghua University, China, 1998.

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Incorporation of Sustainability Education into the Ammonia Synthesis Process Design of the Chemical Engineering Senior Design Course

Sustainability has become a key subject in chemical engineering (ChE) practice, largely due to the challenges such as natural resource depletion, greenhouse gas emission, economic globalization, increasingly stringent environmental regulation, etc. To incorporate the concept into ChE education, the ABET, Inc. has listed sustainability as a crucial element in engineering curricula and stated that "Design of environmental engineering systems that includes considerations of risk, uncertainty, sustainability, life-cycle principles, and environmental impacts." [1]. The senior capstone process design course is a key educational component to fulfill the goal, as it could integrate sustainable subjects into the ChE undergraduate curriculum such as sustainable resources, biomass, energy efficiency, design standards and regulations, process safety, etc.

Decades of efforts have been made by introducing sustainability concepts and tools in the engineering curricula. Allen and Shonnard [2] summarized a body of knowledge as a perspective on sustainability in ChE by three elements: framing the challenge, assessment and design, and systems perspectives. Allen et al. [3] reviewed the progress of the sustainability education and discussed the prospects for future transformations, such as including sustainability modules as supplements into ChE core courses instead of introducing elective courses. Recently, Amini-Rankouhi and Huang [4] shared their educational experience by introducing sustainability manufacturing into process design course. Students were asked to discuss with their teams to select the most appropriate sustainability indicators to assess the design.

In this paper, more efforts in sustainability education have been made in the undergraduate capstone design course, specifically to address the following challenges:

(1) identify new process technologies to design with sustainable features, such as biomass, renewable energy, novel business model, etc;
(2) develop sustainability assessment and analysis methods to merit the sustainable features in a quantitative way;
(3) fill the gap between university study and real-world environment, as well as the gap between existing technology status and future development.

Three approaches have been implemented into the Process Synthesis and Design II to address the challenges in sustainability education:

(1) introduce the wind-based water electrolysis technology into ammonia synthesis design, in addition to the traditional CF-Braun technology;
(2) extend the techno-economic analysis to incorporate emission penalty, renewable resource credit, transportation cost, modular manufacturing discount, as well as safety/control concerns;
(3) invite industrial experts to the final presentation and review the design from various aspects.

After two years implementation, it has demonstrated that the students could gain the insights of the new sustainable process technologies more effectively.

Scope of Design

Two ammonia synthesis processes are designed in parallel: one is the traditional CF-Braun technology (Figure 1), the other is an emerging distributed wind-based water electrolysis technology (Figure 2). In the CF-Braun process, natural gas and steam are the raw materials to form hydrogen via steam reforming and water gas shift reactions. The nitrogen is introduced in the air at the second reformer where the oxygen is consumed via partial oxidation reforming. After amine system, methanation, cryogenic separation, and compressing, the hydrogen and nitrogen are purified and compressed for the ammonia synthesis. After the Haber-Bosch reactor, the unreacted feeds are separated and recycled back. The ammonia would be purified further to obtain the 99.9% liquified ammonia as the product at 1500 tonne/day.

In the distributed wind-based water electrolysis technology, the wind turbines generate electricity which is consumed locally to produce hydrogen via water electrolysis. The nitrogen is separated from the air through the membrane separation units. The oxygen from both water electrolysis and air separation is the by-product. Then the hydrogen and nitrogen are mixed in a 3:1 mole ratio, compressed, and produce ammonia in the reactors. Due to the limit of the wind-based power generation at certain area, each plant capacity at that area would be limited as well. In our study, each plant has 8.2 tonne/day ammonia capacity with totally 184 identical plants to achieve the same 1500 tonne/day as the traditional one. Those plants would be distributed according to the wind turbine locations. Then the liquified ammonia could be transported to a centralized storage unit [5][6][7].

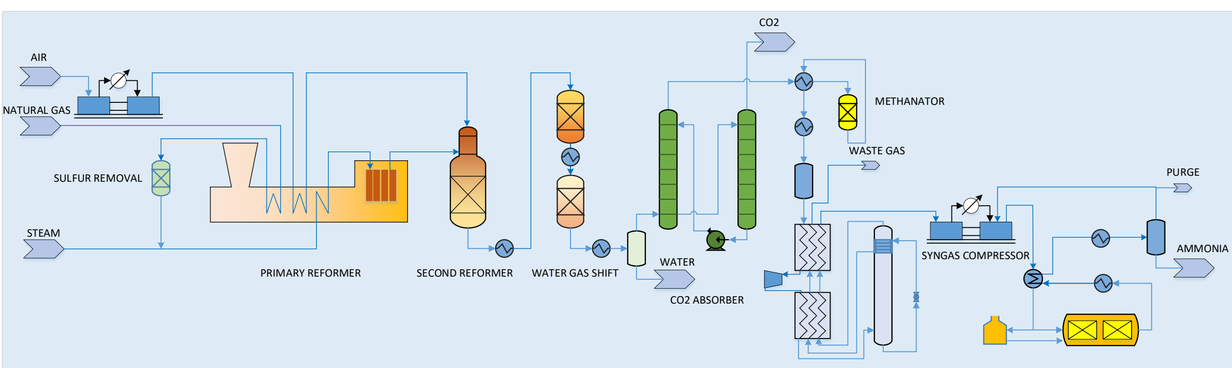

Figure 1. *Traditional CF-Braun ammonia synthesis process.*

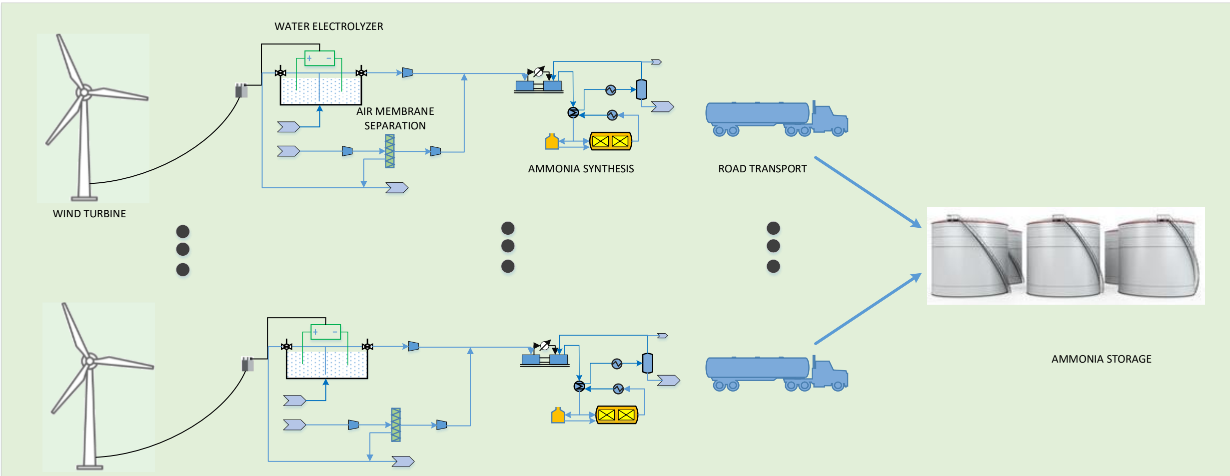

Figure 2. *Distributed wind-based water electrolysis ammonia synthesis process.*

The design procedure includes:

(1) process simulation on software (e.g. Hysys, PROII) to obtain mass and energy balance data;
(2) heat exchanger network design using pinch technology;
(3) equipment sizing (e.g. reactor, vessel, compressor, column, heat exchanger, etc.);
(4) capital and operational cost estimation;
(5) financial analysis (e.g. breakeven cost at 10% interest rate, sensitivity analysis at various raw material or utility cost).

Extended Techno-Economic Analysis of Sustainability Assessment

Techno-economic analysis (TEA) is a methodology framework to analyze the technical and economic performance of a process, product or service. TEA normally combines process modeling, engineering design and economic evaluation [8]. The extended TEA provided in the design class is to address the sustainable features of the novel process to economic performance. Therefore, the merits of the sustainability would be accountable and comparable to the other processes on the same basis [9].

The extended TEA framework is shown in Figure 3. As the basis, the processes are simulated on the fundamental knowledges in thermodynamics, transport phenomena, reaction kinetic models, phase equilibrium, etc. Commercial software is introduced to facilitate the simulation such as Aspen Plus, HYSYS, PROII, etc. The simulation outcomes are the mass & energy balance results which provide the foundation of the evaluation framework.

Then an EXCEL-based evaluation platform is developed to link the simulation results to the economic assessment. It includes the traditional TEA in three parts: (1) capital cost estimation of major equipment and installation, (2) cost of manufacturing estimation of raw materials, labor, utility, waste and maintenance, and (3) financial analysis. Besides the traditional ones, the framework intends to extend the evaluation domain to environment, logistics, society, safety, etc.

By doing so, the merits of the new emerging technologies such as biomass related process, solar or wind-based energy use, distributed modular plant, etc. could be highlighted with more comprehensive criteria. Therefore, various technologies would be quantitatively compared and analyzed under a consistent, traceable platform. In the environment domain, the models would include life cycle analysis, greenhouse gas emission, waste treatment, etc. In the logistic domain, the scheduling and distribution would be studied. In the society domain, more human and community related issues would be involved with quantitative evaluations.

The extended TEA framework makes it possible to perform various studies, including but not limited to (1) multi-objective evaluation of different kinds of technologies, (2) sensitivity study of key parameters in design, and (3) optimal process design by case study or multi-objective optimization. Note that since the framework starts from the fundamental simulation, all the evaluations could be linked to the detailed process and bring insights for the process design.

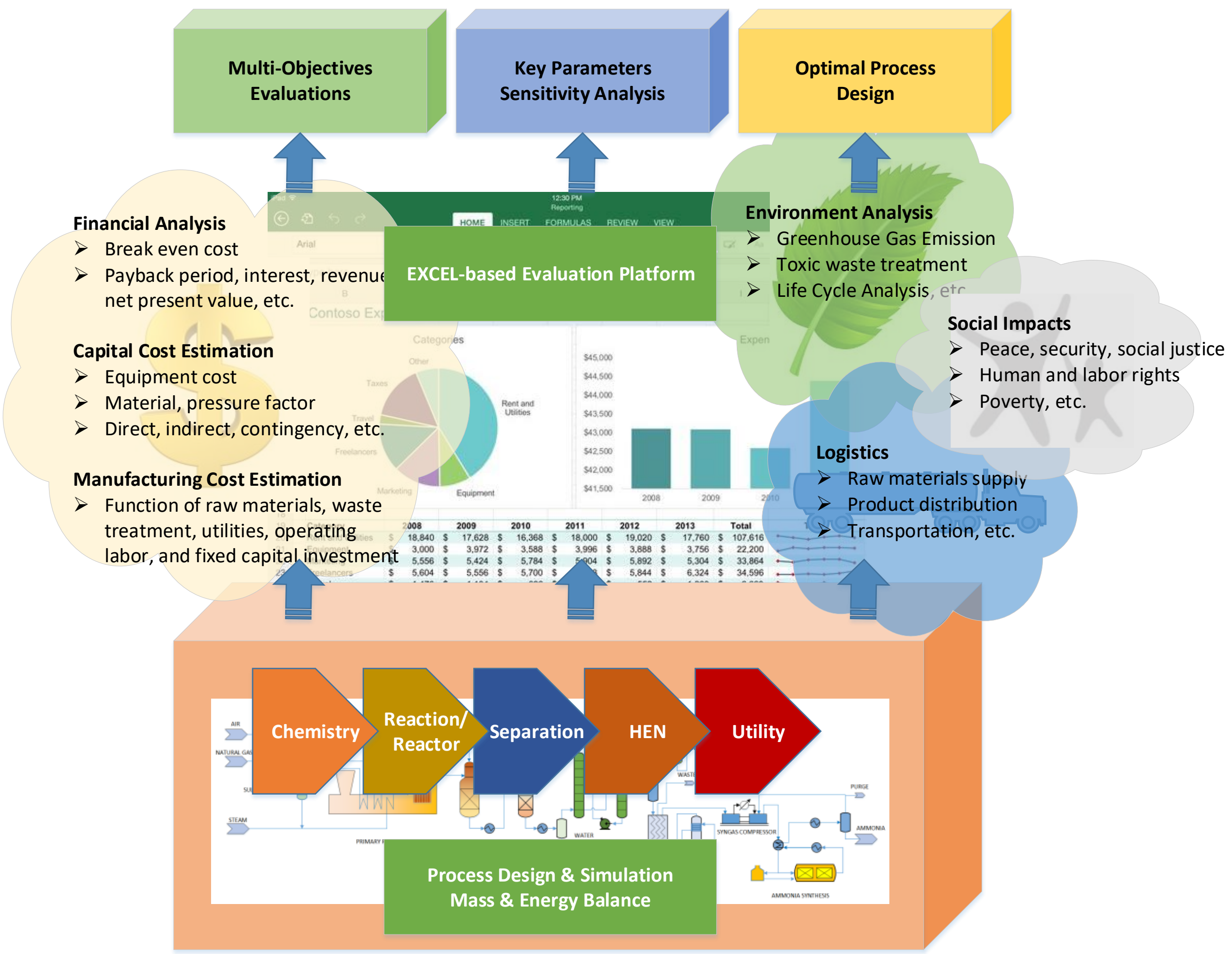

__Figure 3.__ Extended TEA of Sustainability Assessment.

Sustainability Assessment Results

Some design results with sustainability assessment are summarized to show the effectiveness of the extended TEA method. In Table 1, the TEA shows the traditional CF-Braun process needs fixed capital investment (FCI) about 214 USD in million ($214MM), cost of manufacture (COM) about $205MM per year. The breakeven price of ammonia at 10% return rate is about $495/tonne ammonia. This price is similar to the current market price since the majority of ammonia comes from the traditional natural gas-based technologies.

Table 1

TEA results of designed processes

Item	Traditional CF-Braun process	New wind-based (traditional TEA)	New wind-based (extended TEA)
FCI (MM$)	214	850	301
COM (MM$/y)	205	543	298
Price ($/tonne ammonia)	**495**	**1406**	**563**

For the new distributed wind-based water electrolysis ammonia synthesis process, if only the traditional TEA is applied which has no sustainability assessment, the FCI of the total 184 plants is about $850MM. This is because the smaller plant capacity would bring higher capital cost per unit product. The COM of all the plants is about $543MM/year largely due to the much higher energy cost of the electricity compared to the natural gas. As a result, the breakeven price is $1406/tonne ammonia, which is almost three times more than the traditional technologies. Therefore, it seems there is no chance for the emerging technology to compete with the existing ones.

However, if the extended TEA is applied to account the merits of the sustainable features, it would show how the merits reduce the breakeven ammonia price of the new technology. Several case studies are performed in Table 2:

(1) One of the most advantages is the zero CO_2 emission from the wind-based water electrolysis technology. In the traditional one, all the carbon element in the natural gas feed would be converted to CO_2 and releases to the environment. Even the CO_2 is used to produce urea as a fertilizer, it would be converted back and release in the farm land. Therefore, from a life cycle point of view, the traditional process produces 2.312 tonne CO_2 per tonne ammonia. If the CO_2 credit/tax is $30/t$CO_2$, the breakeven price of the new process would be reduced by $69/t$NH_3$. If the CO_2 credit/tax is $50/t$CO_2$, the breakeven price would be reduced by $116/t$NH_3$.

(2) The distributed plants use the renewable and low-value resources that are widely available at local scales (e.g. wind, solar). By converting the electricity into ammonia, it saves the energy loss in transmission and provides operation flexibility, resource independence, price stability, and supply chain robustness. Therefore, the electricity cost in the water electrolysis could be much lower than the industrial one. If the cost is 20% less, then the breakeven price would be reduced by $109/t$NH_3$. If the cost is 50% less, then the ammonia price would be $273/t$NH_3$ less.

(3) Modular fabrication and construction could be applied to the distributed plants. Since the skid-mounted plant could be manufactured in-house and then shipped to the remote area, the engineering and manufacturing cost could be much less compared to an onsite construction.

(4) One active research area is low pressure ammonia synthesis, which reduces the reaction pressure from >150 bar to ~20 bar [10]. It would reduce the compressor capital cost and compressing power, as well as enhance the process safety issue.

(5) Both water electrolysis and air separation would produce oxygen as a byproduct. If the oxygen could be sold, the oxygen credit would reduce the ammonia price by $35/tNH3 with $20/tO2.

Table 2

Sustainability assessment results

Items	Price change ($/tonne ammonia)
Emission reduction CO2 credit ($30/tCO2)	-69
Emission reduction CO2 credit ($50/tCO2)	-116
Wind-based electricity discount (20% discount)	-109
Wind-based electricity discount (50% discount)	-273
Modular manufacturing (FCI 20% discount)	-123
Modular manufacturing (FCI 50% discount)	-306
Low pressure reactor	-154
Oxygen by-product credit ($20/tO2)	-35

If the new process achieved all the sustainable potentials, the extended TEA would give FCI at $301MM, COM at $298MM, and the ammonia breakeven price around $563/tNH3. This is even comparable to the traditional CF-Braun process ($495/tNH3) in this study. Therefore, the wind-based distributed technology shows a promising direction by accounting sustainability in the extended TEA framework.

Course Description and Pedagogical Approaches

The process design project is for ~30 senior students to take 15 weeks to accomplish. One project manager and one associate manager are selected by volunteering and voting. The rest are divided into two big groups, one for each process. Every week, we have group meeting to present the design work with Q&A. On week 15, several industrial experts are invited to review the whole design project in terms of PFDs, presentations, report, and Q&A.

A number of pedagogical approaches have been applied along the teaching as summarized in Table 3.

Table 3

Pedagogical approaches applied in the process design course

Approach	Definition	Application

Integrated Learning	Learning brings together content and skills from more than one subject areas	The extended TEA brings more evaluation areas such as environment, logistics, society, safety, etc.
Inquiry Learning	Learning is directed by questions, problems, or challenges that students work to address.	The weekly group meeting with Q&A would give students directions accordingly.
Experiential Learning	Learning provides experience beyond the classroom. Addressing real world issues and problems	The two process technologies are both from real-world practices. Inviting the industrial review panel would help the students to gain experience and increase their visibility to the job market.
Co-operative Learning	Group and cooperative learning strategies are a priority.	The class is divided into groups with project managers. Each group works together with weekly meetings. The peer review would assess their team work performance.
Peer Teaching	Provides opportunities for students to actively present their knowledge and skills to peers and/or act as teachers and mentors.	The weekly meeting is a good place for students to learn from other groups. Each student could have the overall picture of the design project.
Case Studies	Case studies are thorough descriptions of real events from real situations that students use to explore concepts in an authentic context.	In the sustainability assessment, case studies are applied to cover the possible range (e.g. CO2 credit). It also brings insights to students on how sensitive of each sustainable feature to the economic results.
Open-Ended Instruction	Lessons are structured so that multiple/complex answers are possible.	By comparing the traditional technology to the new sustainable one, the students would know there is no simple Yes or No answer. It depends on complex factors such as technology maturity, policy, market, geographical conditions, etc.
Assessment & Evaluation of Student Learning	Tools are provided that help students and teachers to capture formative and summative information about students' learning and performance.	Self-assessment, peer-assessment, and industrial panel review are provided for assessment (see next section).

Assessment & Evaluation of Student Learning

By introducing the sustainability education in the process design course, the student learning outcomes could be extended to the following three:

(1) Students will learn classical process design methods, including (but not limited to) process simulation, heat exchanger network design, equipment sizing, cost estimation, techno-economic analysis, etc.
(2) Students will learn basic concepts of industrial sustainability and use sustainability assessment and analysis methods to design novel chemical processes.
(3) Students will learn how to compare the novel sustainable processes to the traditional ones and merit the sustainability in a quantitative way.

To assess and evaluate the student learning, three assessments have been implemented at the end of the project: (1) self-assessment, (2) peer-assessment, and (3) industrial review panel assessment. From the assessment results, the new teaching efforts have fulfilled the ABET's requirements and been highly evaluated by both the students and the industrial reviewers.

In the self-assessment, all the senior students are required to complete a self-assessment of their ability to attain the educational outcomes of the Chemical Engineering Program. A short answer with a score would be given for each ABET student outcomes as below:

a) an ability to apply knowledge of mathematics, science, and engineering
b) an ability to design and conduct experiments, as well as analyze and interpret data
c) an ability to design a system, component, or process to meet desired needs within realistic constraints such as economic, environmental, social, political, ethical, health and safety, manufacturability, and sustainability
d) an ability to function on multi-disciplinary teams
e) an ability to identify, formulate, and solve engineering problems
f) an understanding of professional and ethical responsibility
g) an ability to communicate effectively
h) the broad education necessary to understand the impact of engineering solutions in a global economic, environmental and societal context
i) a recognition of the need for, and an ability to engage in life-long learning
j) a knowledge of contemporary issues
k) an ability to use the techniques, skills, and modern engineering tools necessary for engineering practice.

The score is from 1 to 5: 1 means "achieved outcome" and 5 means "room for progress". For the student outcome (c) which is directly related to the sustainability education, the average score has been improved from ~1.3 to almost 1.0 before and after this new design project. The students also give very positive comments on the effort, such as "very interesting to compare the two processes", "learned a lot about the new technology", "give us insights of the sustainability". Two senior students have also published a paper with the author about the extended sustainability assessment framework. Note that the a-k criteria have been supplanted by student outcomes 1-7 in the current EAC-Criteria[1]. The author will update the assessment questions accordingly.

In the industrial review panel assessment, three categories are related to the sustainability:

- Ability of cost estimation and economic analysis
- Ability of understanding environmental and process hazards analysis
- Awareness of ethical, societal and quality concerns.

Most of the scores are between 1 (Exemplary) and 2 (Proficient). The efforts in the sustainability education have drawn a lot of attention by the industrial experts. One senior engineer has been working on cost estimation for 20+ years. He gives high remarks on this work and is willing to share his experience to our students. Two of them are very interested in the assessment method and doing some further study with the author. Inviting the industrial review panel would also help the students to gain experience and increase their visibility to the job market. Every year, we have several students who have received job offers from the review panel members' companies.

Summary

In this paper, three approaches have been implemented into the CHE senior design course to address the challenges in sustainability education: (1) introduce the wind-based water electrolysis technology into ammonia synthesis design, in addition to the traditional CF-Braun technology, (2) extend the techno-economic analysis to incorporate emission penalty, renewable resource credit, transportation cost, modular manufacturing discount, as well as safety/control concerns, and (3) invite industrial experts to the final presentation and review the design from various aspects.

After two years implementation, it has demonstrated that the students could gain the insights of the new sustainable process technologies more effectively. By comparing the designs with extended assessment method, the students could study the pros and cons in a broader scope with quantitative results. Introducing the industrial review panel would help the students to gain experience and increase their visibility to the job market. As a result, the new teaching efforts have fulfilled the ABET's requirements and been highly evaluated by the students' evaluation and reviewers' comments.

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