Modular Teaching and Open Ended Design Projects

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ABSTRACT

Some latest employment surveys show that chemical engineers are working in more and more diverse industries manufacturing specialty and commodity products; they need to understand property-structure relationships using chemistry, biology, and physics. Therefore, modular teaching with open ended design projects can provide a means of responding to diverse and fast changing course contents and learning/teaching objectives. This study presents the experience on modular teaching integrated with the Aspen Plus simulator and discusses open ended plant design projects in the Department of Chemical Engineering at University of Nebraska Lincoln. The projects discussed is the conversion of available carbon dioxide and hydrogen into methanol or/and ammonia. The hydrogen comes from electrolysis of water using the electricity produced by wind power, while the carbon dioxide comes from power plants as well as ethanol plants. The feasibility of the plants at some assumed production capacities with the available technologies are discussed using the discounted cash flow diagrams of the plants. The economic data used, assumed capacities, and the cost of electrolytic hydrogen have all compounded effects on the feasibility of the plants.

Keywords: Modular teaching, capstone design, open ended design projects

1. MODULAR TEACHING

Chemical Engineering discipline has evolved to embrace biological engineering, and its graduates may work as product and process engineer to define products and processes, understand property-structure relationships using chemistry, biology, and physics. This reemphasizes the constant need for revisions of teaching strategies and instructional materials in capstone design. One of the ways of achieving this goal may be modular teaching technique [1-3]. A module is a well-organized, high quality student text based on clear level, prerequisites and learning objectives of a topic. Modules mainly consist of title page, main text, and end materials; they can accommodate institutional and temporal variations and response to diverse and fast changing learning objectives and to the dynamics of accreditation in engineering education. They also follow new practices, the advancements in technology, and departmental curricular needs, and contain design practice problems and relevant references. The main text and the practice problems help students to transfer and synthesize knowledge across the previous courses, provide them with some examples of open-ended problems, and develop strategies in making engineering decisions under uncertainty. However, the effectiveness of modular teaching technique still remains to be assessed properly [1]. The Modules used at the Department of Chemical and Biomolecular Engineering at University of Nebraska Lincon are: M1-Introduction: Design Considerations, M2-Engineering Economics, M-3 Separation Systems, M-4 Heat Transfer and Fluid Flow, M-5 Chemical Reaction Engineering, M-6 Thermodynamics in Design, M-7 Process Synthesis, M-8 Heuristics in Process Design, M-9 Safety, M-10 Green Engineering. The Aspen Plus simulator practices are incorporated into the Modules starting with M-3 Separation Systems. The modules are detailed elsewhere [3].

2. OPEN ENDED DESIGN PROJECTS

The purpose of this design project is to explore the use of the electrolytic hydrogen together with the available carbon dioxide to produce high value chemicals such as methanol and/or ammonia. Electricity produced by wind farms is used in hydrogen production by the electrolysis of water. The carbon dioxide comes from power plants and methanol plants. Using the electrolytic hydrogen and the available carbon dioxide it may be possible to convert and store renewable energy and make use of carbon dioxide if methanol and/or ammonia plant is feasible under current economic conditions and at assumed production capacities with existing technologies. So the open ended design problem is a search of feasible use of the electrolytic hydrogen and carbon dioxide to produce valuable chemicals. We designed and simulated the methanol and ammonia plants with Aspen Plus, and carried out economic analysis by discounted cash flow diagrams for the feasibility of the plants.

2.1 METHANOL PLANT

Process Description

We used the ASPEN PLUS simulator to design and simulate the methanol plant with the RK-SOAVE equation of state property method. The methanol plant uses 786.2 kg/hr hydrogen and 5721.3 kg/hr carbon dioxide, and produces 4169.2 kg/hr and 99-wt% of methanol. The plant operates for 8520 hours/year. We assume that under high pressure (50 bar) and temperature (250°C), there are no side reactions beside the following elementary reaction [4,5]: $CO_2 + 3H_2 = CH_3OH + H_2O$. This reaction is reversible. The forward reaction's conversion is 95% of carbon dioxide. The reaction takes place over a catalyst of $Cu/ZnO/Al_2O_3$ [4]. The cost of major utilities in the form of cooling water, steam, and electricity is around \$1.4 10^6/year. Figure 1 shows the conceptual PDF for the methanol plant with major equipments. The feedstock is at 25^{o}C with a mole ratio of hydrogen to carbon dioxide of 1:3. Stream S6 is the output of the reactor R201 and contains the unused hydrogen and carbon dioxide, as well as the produced methanol and water. This effluent is cooled down to 84°C in E202. The unreacted carbon dioxide and hydrogen are recycled to the reactor in stream S8. The liquid output of F301, at 70^{o}C, is introduced into the stage 24 of the distillation tower T301. The distillate stream 'METHANOL' contains 99.7-wt% of methanol, while the bottoms flow 'WATER' contains 99.7 wt% of water. Table 1 presents the component balance as well as the overall mass and energy balances.

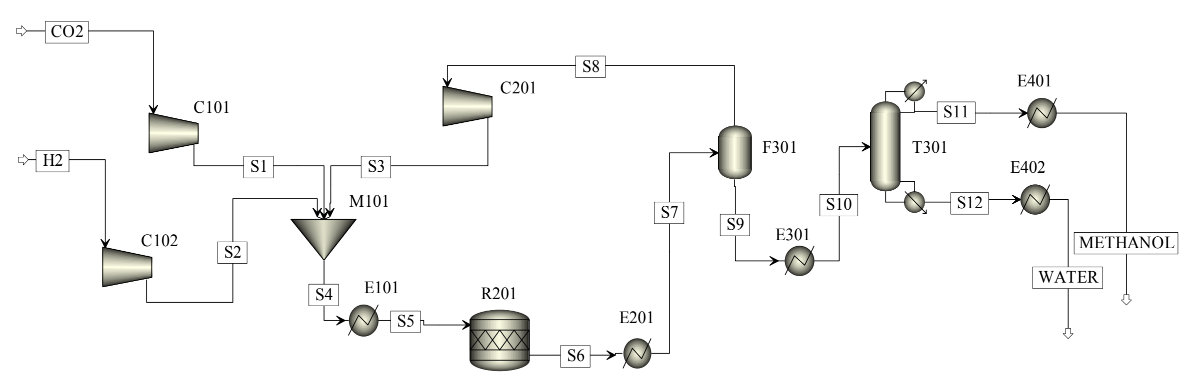

Figure 1. Process flow diagram for methanol plant.

Table 1 Mass and energy balances for the methanol plant

Component balance, kmol/hr	In	Out	Generation
H2	390.0	0.002	-389.8
CO2	130.0	0.05	-129.9
METHANOL	0.0	129.9	129.9
H2O	0.0	129.9	129.9
Mass, kg/hr	6507.5	6507.32	
Enthalpy, Gcal/hr	-12.2209	-16.1622	

Discounted Cash Flow Diagrams (DCFD)

Discounted cash flow diagrams (DCFD) provide the annual cash flows with the time value of the money taken into account [6]. Within the DCFDs it is assumed that the construction time for the plant is one year, the tax is zero, while the interest rate is 5.25%. The useful operation time is 10 years, and the depreciation is based on seven years. The selling price of the primary product methanol is assumed as \$1000.0/MT, while the economic analysis finds the cost of methanol production is \$1400/MT. This result is based on the unit cost of hydrogen by wind power assumed as \$3.5/kg H_2 and at the assumed capacity and using currently available technology for the methanol production. Table 2 displays the data used in the economic analysis.

The DCFD yields a net present value of -\$119.0 10^6 at the end of operation. The sum of working capital, land, and salvage value is fully recovered. The value of net present value (NPV) makes the operation unfeasible. If we can lower the cost of hydrogen from \$3.5/kg to \$1.5/kg and hence the cost of methanol production from \$49.0 10^6 to \$33.0 10^6 the net present value becomes zero, which may make the investment acceptable. Figure 2 shows the DCFD with the new cost of hydrogen.

Table 2 Data used in the economic analysis of methanol plant

Economic data		Economic data	
Bare Module Cost, \$	7.00 10^6	Methanol Production Cost, \$/MT	1400
Fixed Capital Investment, \$	35.00 10^6	Labor, \$/hr each labor	25
Working Capital, \$	7.00 10^6	Number of Labor	15
Land, \$	2.00 10^6	Cost of Labor, \$	3.20 10^6
Salvage, \$	1.40 10^6	Cost of Waste Treatment, \$	0.25 10^6
Revenue, \$	38 10^6	Cost of Raw Material, \$	23.44 10^6
Cost of Production, \$	50 10^6	Cost of Utilities, \$	1.375 10^6
Useful Life of Operation, n , years	10	Carbon Credit, \$/MT CO_2	3.75
Years for MACRS Depreciation, years	7	Revenue for Methanol, \$/MT	1000
Cost of Electrolytic Hydrogen, \$/kg	3.5	Revenue of Water, \$/MT	100
Cost of Carbon dioxide, \$/MT	8.0	Revenue of Carbon credit, \$/year	0.18 10^6

MT: Metric ton

Recommendation

One possible recommendation would be the co-production of methanol with other product which uses methanol as feedstock such as biodiesel, or dimethyl ether, or dimethyl carbonate.

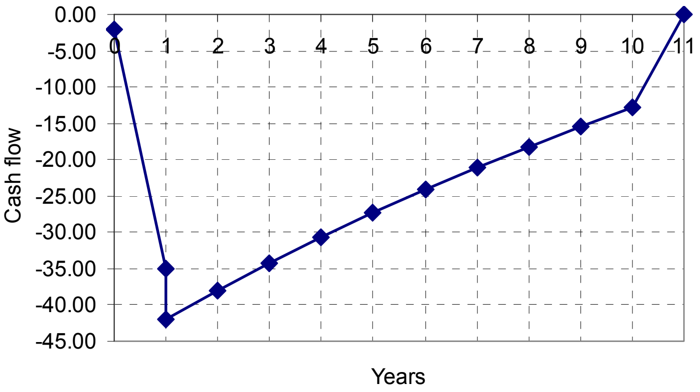

Figure 2. Discounted cash flow diagram for the methanol plant with electrolytic H_2 cost of $1.5/ kg H_2.

2.3 AMMONIA PLANT

Process Description

The ammonia process is simulated by the Aspen Plus simulator with RK-SOAVE equation of state property method. The ammonia plant uses 9071.5 kg/hr hydrogen and 42.48.3 kg/hr nitrogen, and produces 50111.1 kg/hr 99.9 wt % anhydrous ammonia. The plant operates for 8520 hours per year. Air is separated in SEP 101, and the feeds of nitrogen and hydrogen at 20.27 bar are mixed in M101. This mixture is compressed to about 212 bar in compressors C101 and C102. In reactor R201 the ammonia synthesis $3H_2 + N_2 \rightarrow 2NH_3$ takes place at around 556°C and 212 bar with a platinum group metal such as ruthenium. The reactor R201 is a RGIBBS reactor and estimates the equilibrium composition of the reactor by Gibbs free energy minimization. The output of the reactor is conditioned in heat exchangers E202 and E203 and sent to adiabatic flash drums FL301 and FL302, which operate at 203 atm and at 12 bar, respectively. The bottom flow of FL302 is the product ammonia at -26°C and 12.4 bar. Figure 3 shows the conceptual PFD for the ammonia plant with major equipments. The ammonia plant requires electricity, cooling water, steam, and refrigeration as utilities. The flow rate of ammonia is maximized to be 2942.7 kmol/hr and its composition to be 0.99-wt% within the optimization block with constraints. Tables 3 presents the overall mass and energy balances for the ammonia plant.

Table 3 Overall mass and energy balances for the ammonia plant

Component balance, kmol/hr	In	Out	Generation
N2	1501.0	29.5	-1471.4
H2	4500.0	85.5	-4414.4
NH3	0.0	2943.0	2942.9
Overall Balance, kmol/hr	6400.00	3457.0	-2942.9
Mass, kg/hr	63887.2	3887.8	
Enthalpy, Gcal/hr	0.1770	-50.3657	

Discounted Cash Flow Diagrams (DCFD)

The DCFDs are prepared for a ten-year of operation time and a one-year of construction time for the ammonia plant. The tax is zero, while the interest rate is assumed to be 5.25%. The depreciation is based on seven years. Table 4 displays the data used in the economic analysis. The revenue of ammonia is assumed to be \$600.0/MT. The cost of ammonia production is estimated as \$985.0/MT. This result is based on the unit cost of hydrogen by wind power assumed as \$3.5/kg H_2 at the assumed production capacity and using the current technology.

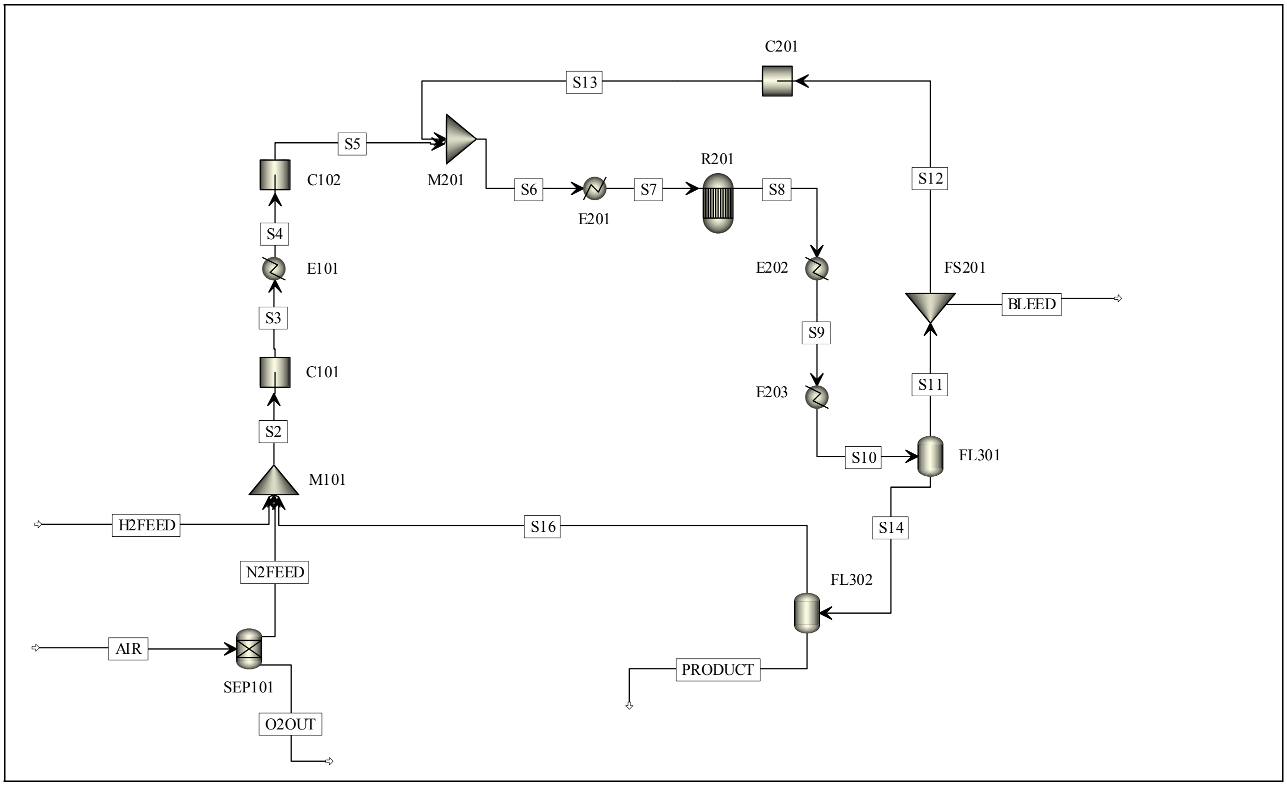

Figure 3 Process flow diagram for the ammonia plant.

Table 4 Data used in the economic analysis of the ammonia plant

Economic data		Economic data	
Bare Module Cost, \$	37,131,000	Cost of Labor, \$	4,260,000
Fixed Capital Investment, \$	185,655,000	Cost of Waste Treatment, \$	1,000,000
Working Capital, \$	37,131,000	Cost of Raw Material, \$	270,690,062
Land, \$	3,000,000	Cost of Utilities, \$	21,301,862
Salvage, \$	7,000,000	Cost of Labor,\$	25
Revenue, \$	310,557,680	Number of Labor	20
Cost of Production,	423,993,268	Cost of Hydrogen, \$/kg H_2	3.5
Revenue of Oxygen, \$/kg O_2	0.05	Cost of Nitrogen, \$/kg N_2	0.5
Revenue of Ammonia, \$/kg NH_3	0.60	Output of Oxygen , kg O_2/hr	12767

The net present value at the end of operation is -\$989.0 10^6. The sum of working capital, land, and salvage value is fully recovered. With the current economic data (Table 4), the ammonia plant is unfeasible. If we can reduce the cost of hydrogen production from \$3.5/kg to \$2.0/kg the NPV becomes zero. Figure 4 shows the DCFD with the new cost of hydrogen production of \$2.0/kg. Also, if the revenue of ammonia increases from \$0.60/kg to \$0.92/kg then the NPV becomes zero with the hydrogen cost of \$3.5/kg.

Recommendation

One of the possible recommendations would be the co-production of ammonia and urea as fertilizers.

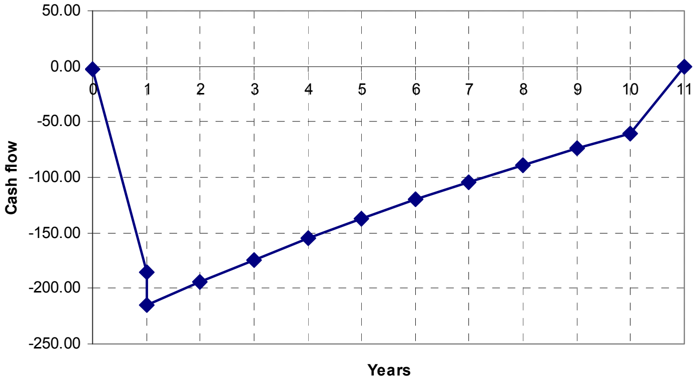

Figure 4 Discounted cash flow diagram for the ammonia plant with electrolytic H_2 cost of \$2.0/kg H_2.

Table 5 summarizes the effects of the cost of electrolytic hydrogen production and the revenue of methanol and ammonia on the NPV. The net present value will be equal to zero if the hydrogen production cost is reduced from \$3.5/kg H_2 to \$1.5/kg H_2, or the methanol revenue is increased from \$1.0/kg to \$1.46/kg at the assumed production capacity. On the other hand, the net present value will be equal to zero if the hydrogen production cost is reduced from \$3.5/kg H_2 to \$2.0/kg H_2, or the ammonia revenue is increased from \$0.6/kg to \$0.92/kg at the assumed production capacity for the ammonia plant.

Table 5 Effects of the cost of electrolytic hydrogen and revenues of methanol and ammonia on the NPV.

Cost of hydrogen, \$/kg	Revenue of methanol, \$/kg	Cost of methanol production, \$	Methanol plant Net present value, \$
3.50	1.00	50 10^6	-119.0 10^6
1.5	1.00	34 10^6	0.0
3.50	1.46	50 10^6	0.0
	Revenue of ammonia, \$/kg	Cost of ammonia production, \$	Ammonia plant Net present value, \$
3.50	0.60	424 10^6	-989.0 10^6
2.00	0.60	288 10^6	0.0
3.50	0.92	424 10^6	0.0

3. OTHER USES OF CARBON DIOXIDE AND HYDROGEN

Carbon dioxide is a very stable molecule and hence energy is generally necessary to drive the desired conversion. Thus high temperatures, extremely reactive reagents, electricity, or the energy from photons may be necessary to carry out carbon dioxide reactions. Reactions of carbon dioxide are dominated by nucleophilic attacks at the carbon, which result in bending of the O-C-O angle to 120°; i.e. hydroxide attack on carbon dioxide to form bicarbonate. Carbon dioxide may be converted to: (a) ammonia/urea $C(O)(NH_2)_2$, and (b) sodium bicarbonate ($NaHCO_3$). Carbon dioxide is also an intermediate in organic syntheses for melamine and urea resins productions. Supercritical carbon dioxide is a hydrophobic solvent which can replace organic solvents in some applications; solvent costs may be reduced and emission of toxic organics can be reduced. Fuel cells convert hydrogen to electricity, heat, and water.

4 DISCUSSION AND CONCLUSIONS

Modular teaching and open ended design projects may enhance student's skill of transferring and synthesizing knowledge across courses, and decision making under uncertainties. Modular teaching can accommodate diverse and fast changing course contents and learning/teaching objectives.

Open ended design projects considered in this study analyze the use of electrolytic hydrogen with the available carbon dioxide to produce valuable chemical products, such as methanol, ammonia, and/or sodium bicarbonate. The cost of electrolytic hydrogen strongly affects the economics of the methanol and ammonia plants at the capacities assumed in this study and using currently available technologies. The methanol plant is economically feasible if the electrolytic hydrogen cost is less than \$1.5/kg hydrogen. The ammonia plant is not favorable under current economic conditions. A feasibility study is needed for sodium bicarbonate production. The analyses at some assumed production capacities with the available technologies show that the economic data, assumed capacities, and the cost of electrolytic hydrogen have all compounded effects on the feasibility of the methanol and ammonia plants. However, changing economic conditions, ongoing research and technological developments could lead to improved efficiencies and cost-effectiveness for the production of hydrogen, methanol, ammonia, and hence the analyses may lead to open ended results.

Worldwide, we use only 110 million tons to produce other chemicals (mainly urea) of the 3500 million tons carbon dioxide we add annually. Therefore it is critical to use carbon dioxide as feedstock for production of other valuable chemicals.

REFERENCES

1. Brusic, S.A., LaPorte, J.E., The Status of Modular Technology Education, Int. Tech, Ed. Assoc. Conf., 1999, Indianapolis, IN.
2. Demirel, Y., Modular Teaching Experience in Capstone Design, AIChE's Annual Meeting, November 7-12, 2004, Austin, TX.
3. Demirel, Y., Modular Teaching and Product Design Projects in Capstone Design ASEE SE Section Annual Conference, April 3-5, 2005, University of Tennessee at Chattanooga, TN.
4. M. Lachowska, J. Skrzypek, Methanol synthesis from carbon dioxide and hydrogen over Mn-promoted copper/zinc/zirconia catalysts. Reaction Kinetics Catalysis Letters, 83 (2004) 269-273.
5. D. Mignard, M. Sahibzada, J.M. Duthie, H.W. Whittington, Methanol synthesis from flue-gas CO2 and renewable electricity: a feasibility study. International Journal of Hydrogen Energy. 28 (2003) 455-464.
6. R. Turton, R.C. Bailie, W.B. Whiting, J.A. Shaeiwitz, Analysis, Synthesis, and Design of Chemical Processes, 2nd edition, Prentice Hall, Upper Saddle River, 2003.