An Integrated Evaluation Method with Application to a New Ammonia Synthesis Process Design

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11/14/2019

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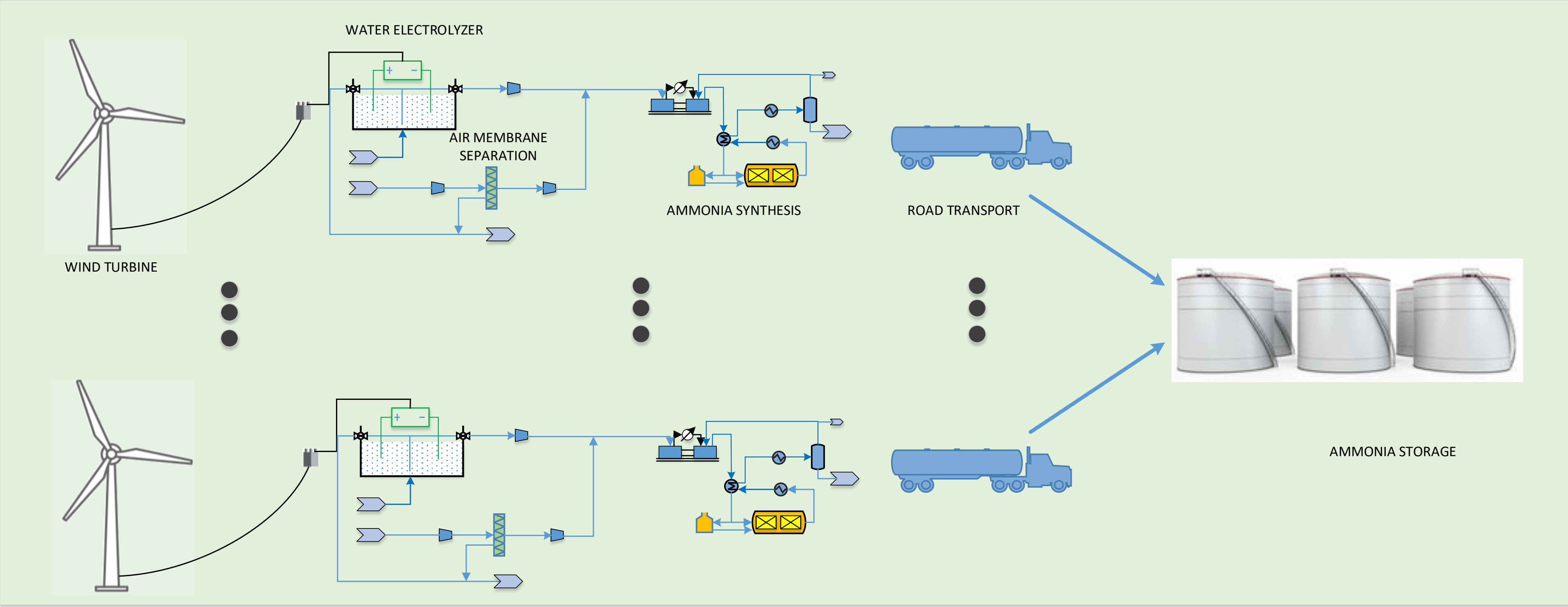
- Motivations
  - Features of new emerging process technologies
  - Challenges in process design and evaluation
- Multi-Objective Multi-Technology (MOMT) Process Design & Evaluation
  - Distributed wind-based water electrolysis for ammonia synthesis
  - Evaluations of the new emerging process features
- Comparison & Discussion
- Summary

Features in New Processes

- Distributed, modularized, and small-scale production
- More flexible, shorter time to market, and better use of distributed renewable raw materials (e.g. biomass) and energy (e.g. solar and wind)



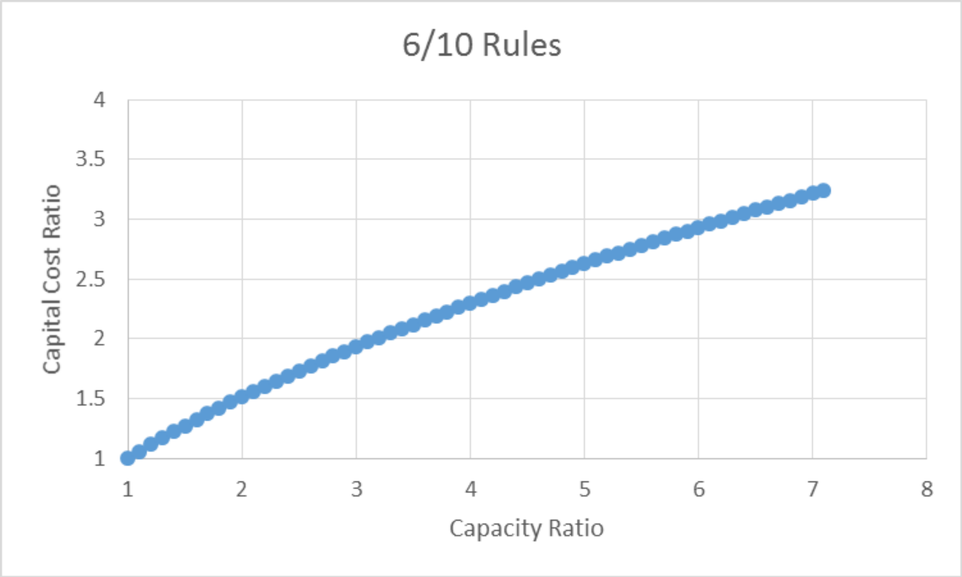
Distributed Wind-based Water Electrolysis for Ammonia Synthesis

Challenges in New Process Design

- Traditional Techno-Economic Assessment (TEA)
  - Capital cost (equipment purchase cost, direct, indirect, etc.)
  - Manufacturing cost (raw materials, utilities, labor, maintenance, etc.)
- Tend to lower the value of the new processes
  - Small-scale would make higher capital cost and lower operation efficiency.

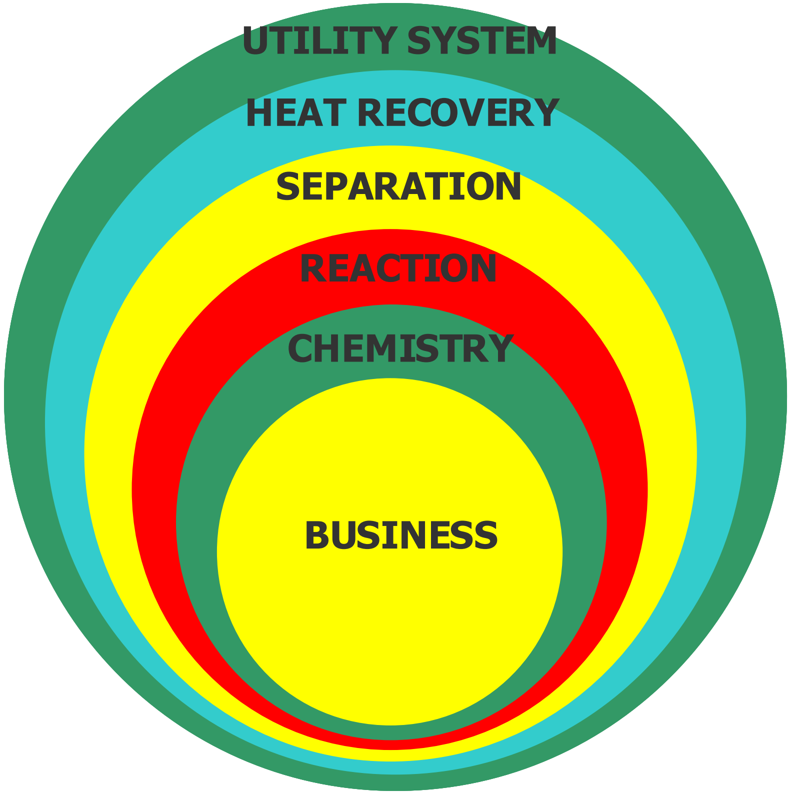
$$\frac{C_a}{C_b} = \left(\frac{A_a}{A_b}\right)^n$$

C – Capital Cost
A – Equipment size or capacity
n – 0.6



Challenges in New Process Design

- Traditional process development procedure /scope



- How to cooperate the new features into the design procedure/scope?
  - e.g. process intensification, emission, renewable energy, HAZOP, life cycle analysis, … etc.
- How to convert to $?
  - Compare designs apple to apple

Extended Scope in Design/Evaluation

Capital Cost
- Modular manufacturing
- Process intensification

IP Position
Mature tech., commercialized?

Environmental Criteria
- Emission penalty
- Waste treatment
- Life cycle analysis
- Toxic materials

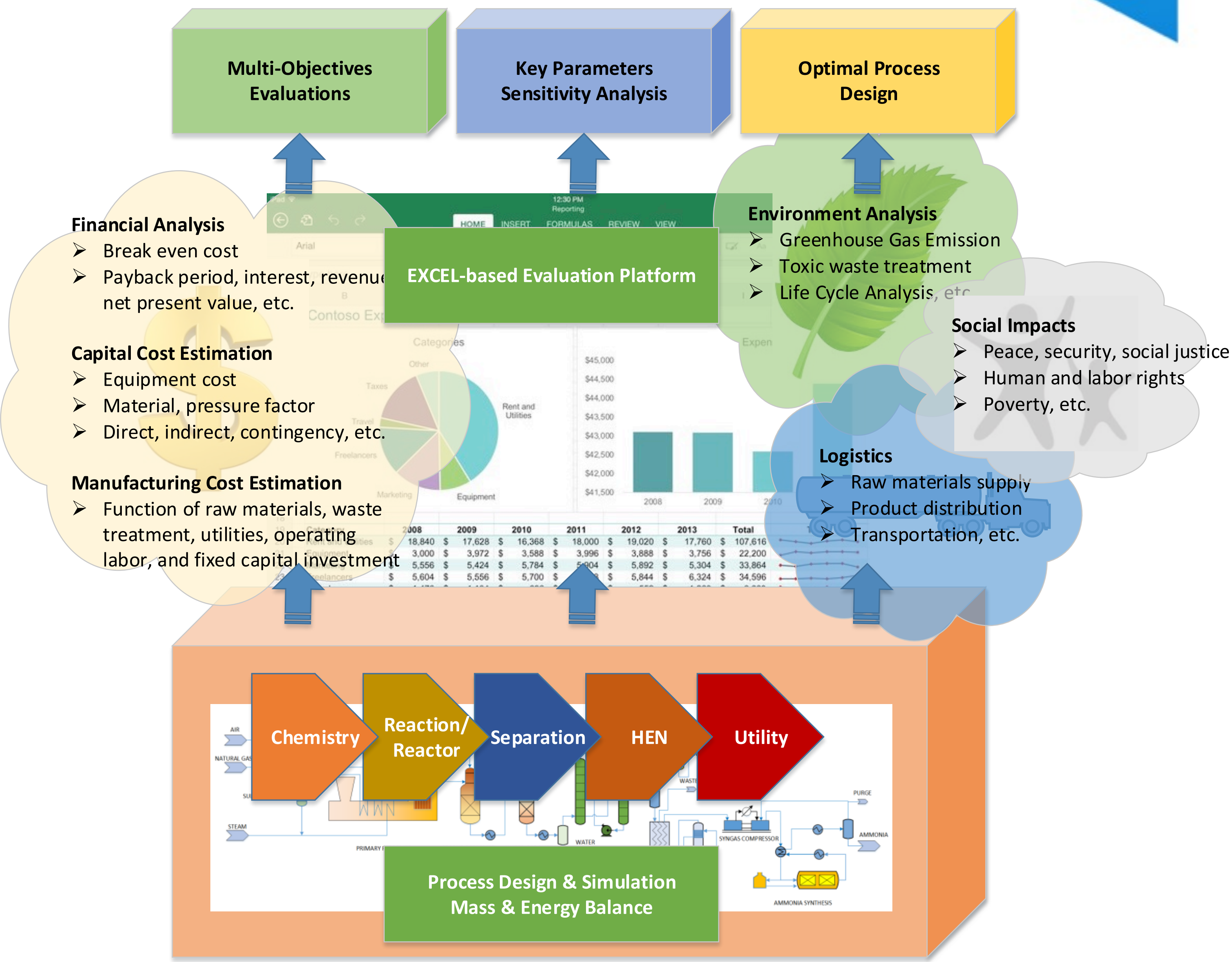
Manufacturing Cost
- Utility system integration (e.g. cogeneration)
- Grid electricity (e.g. peak and valley)

Logistics Criteria
- Scheduling
- Raw materials supply (e.g. biomass)
- Product distribution (e.g. transportation)

Social Criteria
Human rights, poverty, etc.

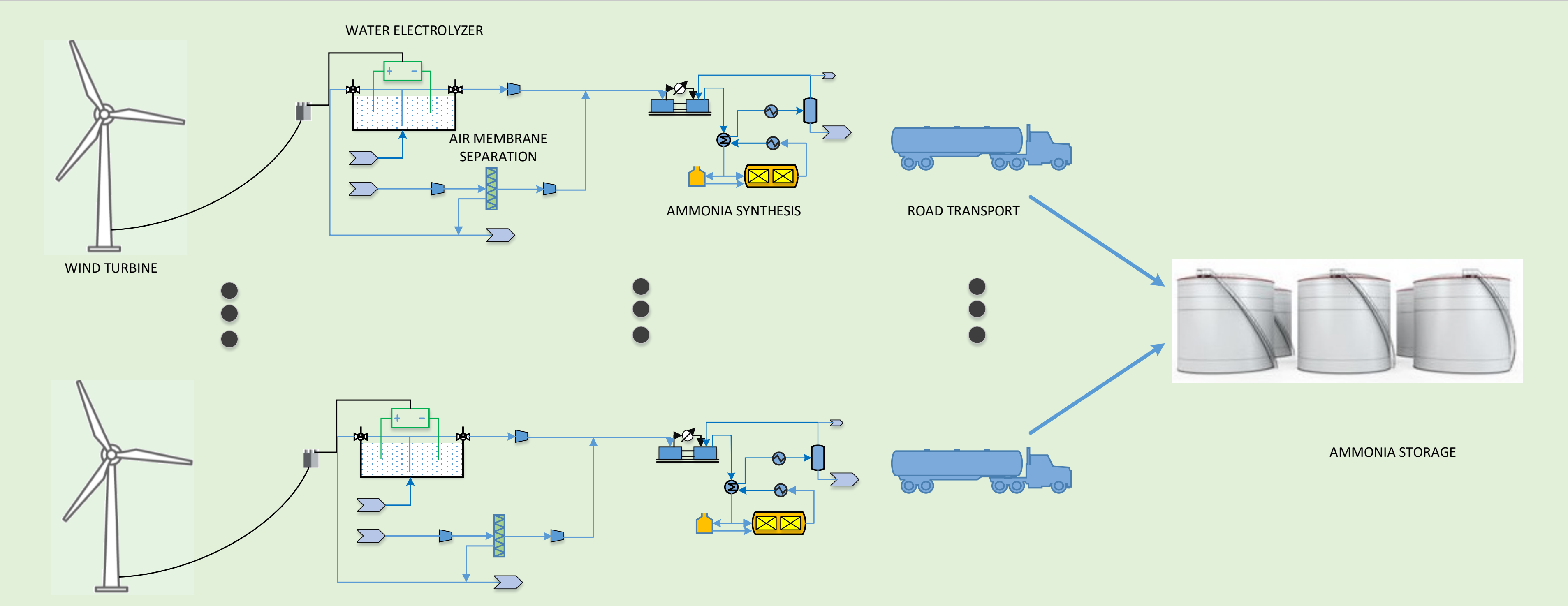
Operation Criteria
HAZOP, flexibility, robust, etc.

MULTI-OBJECTIVE MULTI-TECHNOLOGY (MOMT) FRAMEWORK



Distributed Wind-based Water Electrolysis

- Use the small quantities of low-value resources that are widely available at a local scale (e.g. wind, solar).
- Selling products like fertilizer, energy storage, or fuel; or services like resource independence, price stability, or supply chain robustness.



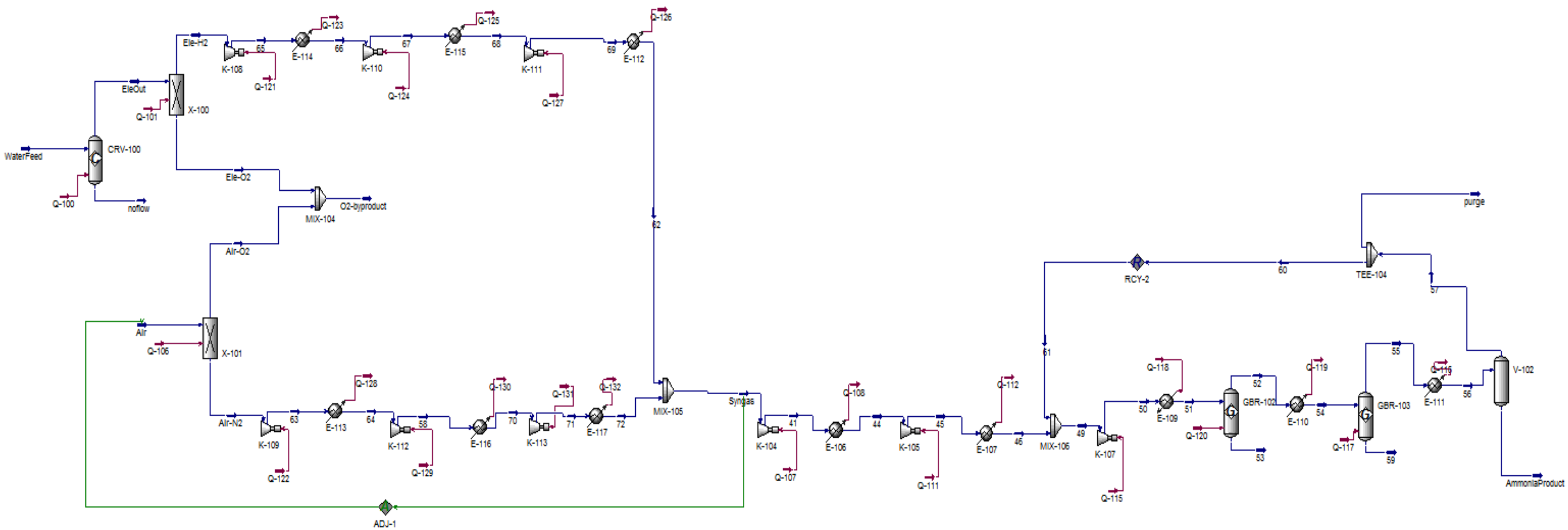
Distributed Wind-based Water Electrolysis for Ammonia Synthesis

Design Specifications

- Electricity generation
  - Wind-based turbine 2.8 MW each plant
- Hydrogen generation
  - Water electrolysis, H_2 production 1500 kg/day (62.5 kg/hr)
  - Electricity consumed 2.5 MW, water consumed 14 tonne/day (0.6 tonne/hr)
- N_2 generation
  - Air membrane separation, N_2 production 7 tonne/day (292 kg/hr)
- Ammonia synthesis
  - Option 1: Traditional Haber Bosch technology, 402 C & 175 bar, 96% overall conversion rate, NH_3 production 8.2 tonne/day (340 kg/hr)
  - Option 2: Low pressure ammonia synthesis, 20 bar, assume the same overall conversion rate.

Process Simulation

- HYSYS-based simulation for Mass-Energy-Balance results.



Name	WaterFeed	EleOut	noflow	Ele-H2	Ele-O2	Air	Air-O2	Air-N2	O2-byproduct
Vapour Fraction	0	1	0	1	1	1	1	1	1
Temperature [C]	20	85	85	85	85	20	20	20	74.92106403
Pressure [bar]	1	1	1	1	1	1	1	1	1
Molar Flow [kgmole/h]	31.19605137	46.79407706	0	31.19605137	15.59802569	13.36263514	2.928555117	10.43408002	18.5265808
Mass Flow [kg/h]	562	562.0280625	0	62.89124058	499.1368219	387.0517872	94.76189853	292.2898887	593.8987205
Liquid Volume Flow [m3/h]	0.563134139	1.338990536	0	0.900258381	0.438732155	0.44509315	8.26E-02	0.362474336	0.521350969
Heat Flow [MW]	-2.483632515	2.25E-02	0	1.48E-02	7.63E-03	-1.08E-03	-6.37E-04	-4.45E-04	7.00E-03
Name	Syngas	41	44	45	46	49	50	51	52

Equipment Sizing & Capital Cost Estimation

- EXCEL-based equipment sizing & capital cost estimation
- Major equipment (electrolyzer, membrane, reactor, vessels, compressors, HXs, etc.)
- Capital cost estimation resources
  - Aspen Economic Analyzer (Icarus)
  - Published cost data of similar equipment/plant (adjusted by scale and time)
  - Vendor's information
- Plant cost estimation
  - f.o.b. purchased cost, bare module, and fixed capital investment (FCI)

Ammonia Synthesis from Natural Gas Base Case Process Flow Diagram & Specifications

ID	Description	Simulation basis	Simulation results	Sizing basis	Sizing results	Costing basis	f.o.b. cost (equipment)	Direct cost
Section 1 - Feed preparation, Reformers, WGS								
R-101	Desulfurizer	Component Splitter, all H_2S is removed.		holdup time 2 min.	Volume (ft3) 70.6; Diameter (ft) 4; Length (ft) 12	using Aspen Process Economic Analyzer (ICARUS)	$266,400	$593,600
R-102	Primary Reformer	Isothermal Gibbs Reactor at 665.6 C.	CH_4 conversion 23%. Duty = 32 MW (115 GJ/h)	(1) A maximum conventional heat flux (21000 btu/ft2/hr) was used to find the total surface area of the tubes. (2) Kinetic model MATLAB code to have catalyst volume.	Kinetic model required more tubes. For a standard tube size (D=4 inches; L= 35 feet), (1) needs 193 tubes, while (2) needs 450 tubes.	The only value for the primary reformer that was available in literature was a cost in the range of $5 million dollars.	n/a	$5,058,380
R-103	Secondary Reformer	Adiabatic Gibbs Reactor, air flow is determined by the CH_4 slip and N_2:H_2 around 1:2	Outlet T = 866 C.	The secondary reformer was sized using literature values from the Jamuna Fertilizer Company.	Volume (ft3) 6713; Diameter (ft) 14.6; Length (ft) 40.1; Thickness (ft) 0.38		$740,800	$973,900

Equipment Sizing & Capital Cost Estimation

New feature

- Modular Manufacturing
  - In-house fabrication and shipping vs. onsite construction
  - Flexible, risk distribution
  - Mass production
  - Maintenance & repair

- Case study
  - 184 distributed plants to have 1500 tonne/day ammonia
  - FCI discount 20% ~ 50% (e.g. engineering, administrative, purchase discount, etc.)

Cost of Manufacturing

- Direct costs, fixed costs, & general expenses

$$COM_d = 0.180FCI + 2.73C_{OL} + 1.23(C_{UT} + C_{WT} + C_{RM})$$

RM = raw materials
WT = waste treatment
UT = utilities
OL = operating labor
FCI = fixed capital investment

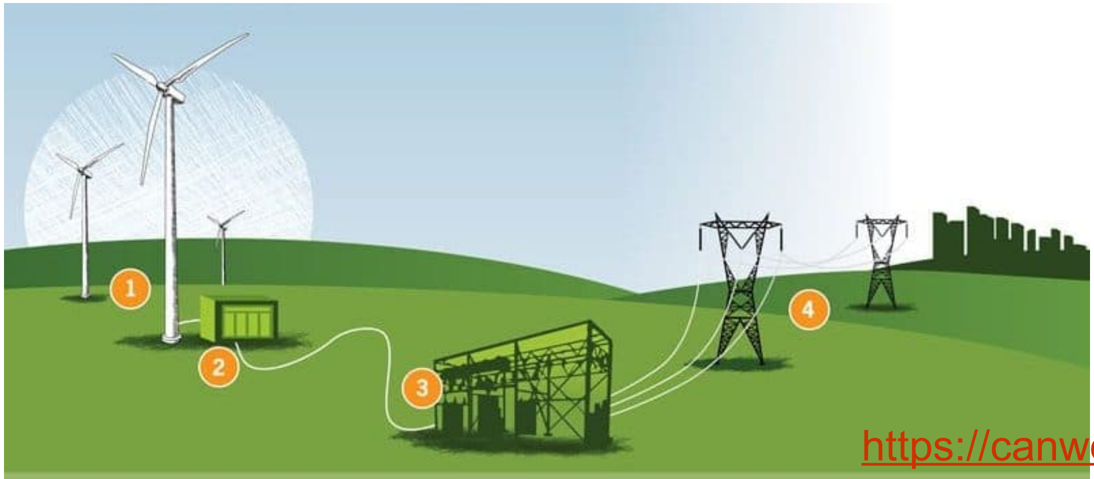
- Base case
  - Raw material: electricity cost for water electrolyzer at \$0.074/kWh
  - Utility: electricity cost for compressing
  - Operating labor: assume \$180,000/each plant

Ref: Turton et al, Analysis, Synthesis, and Design of Chemical Processes (4th Edition), Prentice Hall.

Cost of Manufacturing

New feature

- Wind-based electricity
  - Low-value resource but is widely available at a local scale
  - By converting the electricity into ammonia, it saves the energy loss in transmission and provides operation flexibility of electricity grid
- Case study
  - Assume 20%~50% electricity cost discount by considering transmission loss saving, grid operation, subsidy, etc.



https://canwea.ca/wind-facts/why-wind-works/

Emission Control

New feature

- Zero CO_2 emission from the wind-based water electrolysis technology
  - Even the CO_2 is used to produce urea as a fertilizer, it would be converted back and release in the farm land.
  - Life cycle CO_2 emission of the traditional natural gas HB process: 2.312 tonne CO_2 per tonne ammonia.
- Case Study
  - Apply CO_2 credit/tax to the financial analysis
  - The current central estimate of the social cost of carbon is roughly $40 per ton. (https://www.edf.org › true-cost-carbon-pollution)

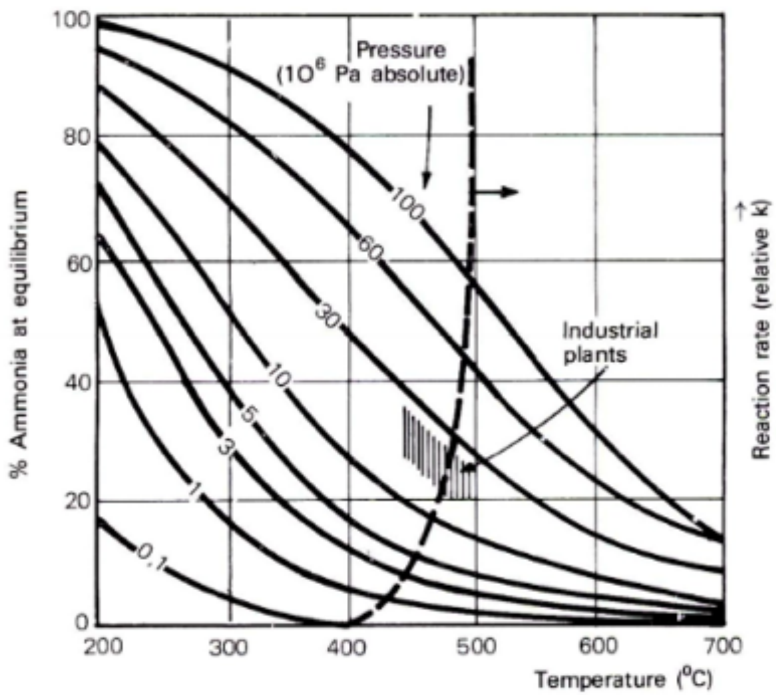
Novel Ammonia Synthesis Technology

New feature

- Low pressure ammonia synthesis (University of Minnesota)
  - Reactive−absorption process for enhanced production of ammonia at reduced operating pressure.

$$N_2 + 3\,H_2 \rightarrow 2\,NH_3 \quad (\Delta H = -92.4\ kJ\cdot mol^{-1})$$

- Case study
  - Reaction pressure is 20 bar
  - Save syngas compressors & compressing power
  - Reactor capital cost and other operating cost are assumed to be the same as HB process

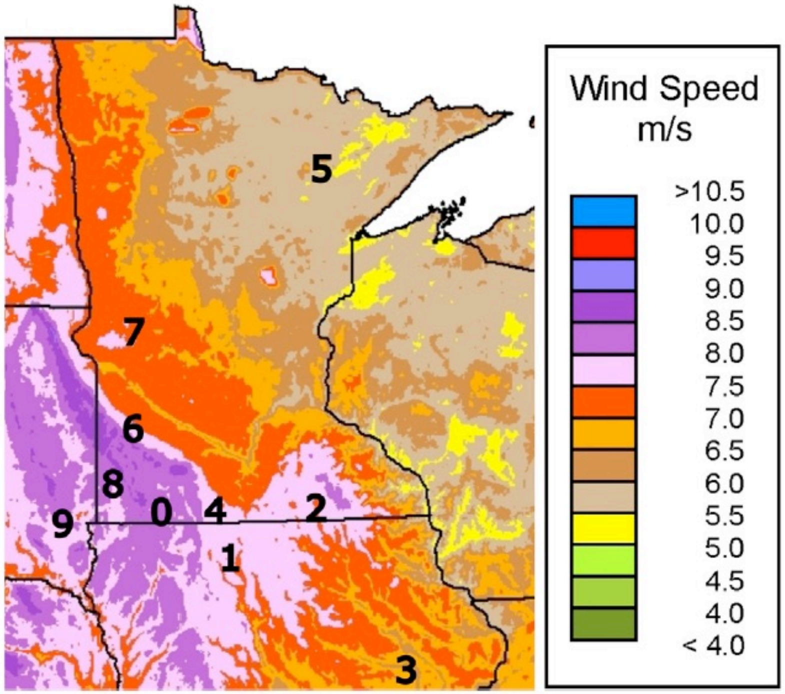


Equilibrium of Ammonia Synthesis

Others

New feature

- O2 credit
  - 1.734 tonne O2 per tonne ammonia. (84% from electrolysis, 16% from air separation)
  - Assume $20/tonne O2
- Logistics
  - Effects of wind capacity, location, plant scale, etc.



Allman, A., Daoutidis, P., Optimal scheduling for wind-powered ammonia generation: Effects of key design parameters. Chem. Eng. Res. Des. (2017)

Financial Analysis

- Generate discounted profitability table (Turton's book)
  - Fixed capital investment & Land
  - Depreciation (MACRS 5 years)
  - Revenue (from NH3 sale price)
  - Manufacturing cost
  - Tax (avg. US tax 26%)
  - Plant life (2 year construction, 10 year operation)
  - Salvage value (assume 7% of FCL)
  - Interest rate (10%)

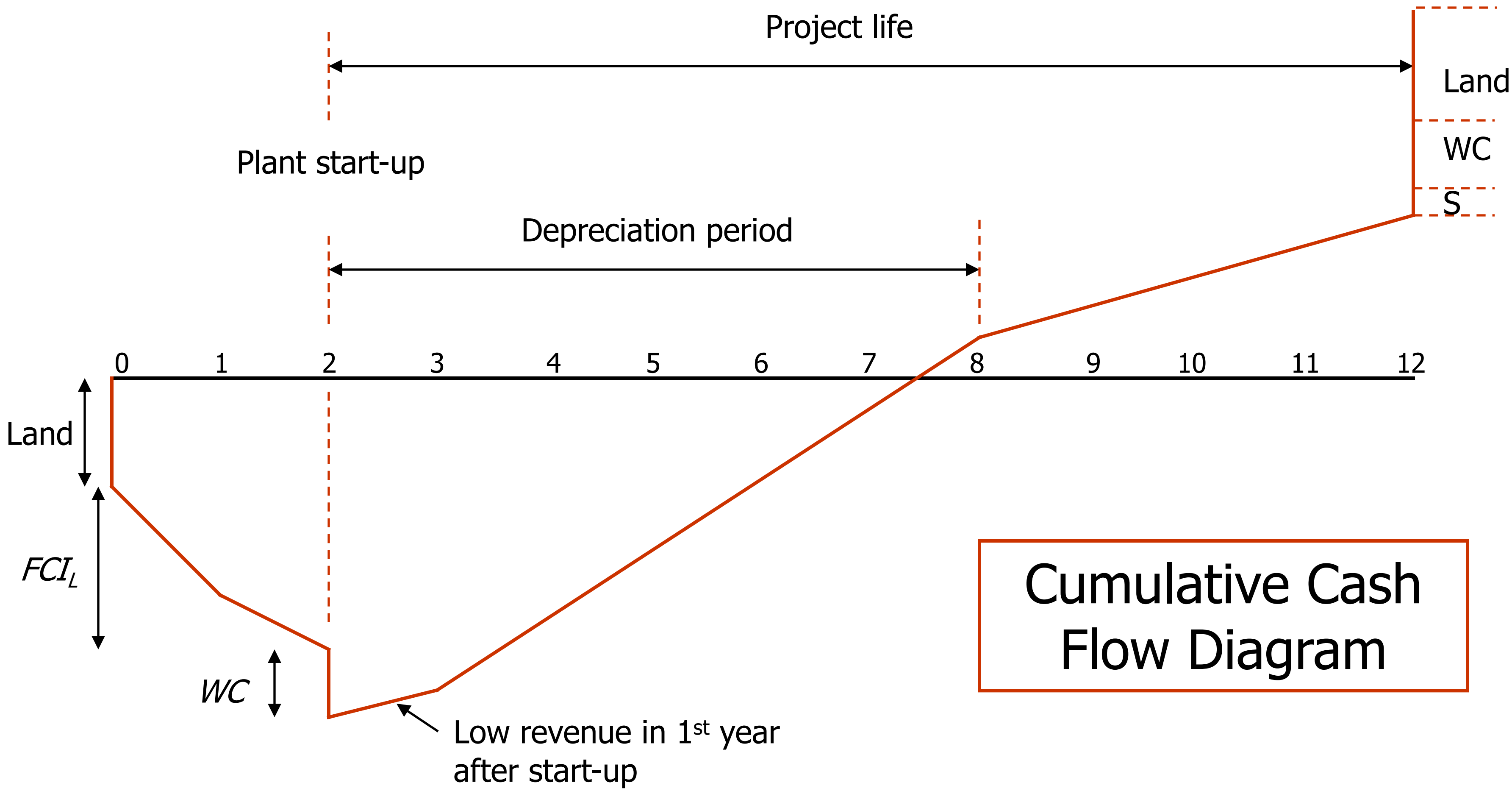
Ammonia Synthesis from Natural Gas Base Case Financial Analysis

Un-depreciation Land Cost	$10,000,000	no cost and area in report, assume.
Fixed Capital Investment (no land)	$204,030,000	in report
1st year FCI	$122,418,000	60% of FCI
2nd year FCI	$81,612,000	40% of FCI
Working Capital	$22,500,000	one month ammonia revenue
Depreciation Method	5-year MACRS	
Ammonia Sale Price $/tonne	$500	
Ammonia Sale Revenue $/yr	$250,000,000	1500tpd, 8000 hour
Cost of Manufacture $/yr	$205,086,306	
Tax Rate	26%	Use average US tax rate
Salvage Value	$14,282,100	assume 7% of FCL
Interst Rate	10%	
Other Information	2 year construction, 10 year operation	

Discounted Profitability Criteria

End of year, k	Investment	dk (depreciation)	FCIL-sum(dk)	R	COMd	(R-COMd-dk)(1-t)+dk	Cash flow	Sum(CF)	Disc CF	Sum(Disc CF)
0	-$10,000,000		$204,030,000				-$10,000,000	-$10,000,000	-$10,000,000	-$10,000,00
1	-$122,418,000		$204,030,000				-$122,418,000	-$132,418,000	-$111,289,091	-$121,289,09
2	-$104,112,000		$204,030,000				-$104,112,000	-$236,530,000	-$86,042,975	-$207,332,06
3		$40,806,000	$163,224,000	$250,000,000	$205,086,306	$43,845,693.65	$43,845,694	-$192,684,306	$32,941,919	-$174,390,14
4		$65,289,600	$97,934,400	$250,000,000	$205,086,306	$50,211,429.65	$50,211,430	-$142,472,877	$34,295,082	-$140,095,06
5		$39,173,760	$58,760,640	$250,000,000	$205,086,306	$43,421,311.25	$43,421,311	-$99,051,565	$26,961,218	-$113,133,84
6		$23,504,256	$35,256,384	$250,000,000	$205,086,306	$39,347,240.21	$39,347,240	-$59,704,325	$22,210,491	-$90,923,35
7		$23,504,256	$11,752,128	$250,000,000	$205,086,306	$39,347,240.21	$39,347,240	-$20,357,085	$20,191,356	-$70,732,00
8		$11,752,128	$0	$250,000,000	$205,086,306	$36,291,686.93	$36,291,687	$15,934,602	$16,930,340	-$53,801,66
9			$0	$250,000,000	$205,086,306	$33,236,133.65	$33,236,134	$49,170,736	$14,095,365	-$39,706,29
10			$0	$250,000,000	$205,086,306	$33,236,133.65	$33,236,134	$82,406,869	$12,813,968	-$26,892,32
11			$0	$250,000,000	$205,086,306	$33,236,133.65	$33,236,134	$115,643,003	$11,649,062	-$15,243,26
12	$32,500,000		$0	$264,282,100	$205,086,306	$43,804,887.65	$76,304,888	$191,947,891	$24,313,089	$9,069,82

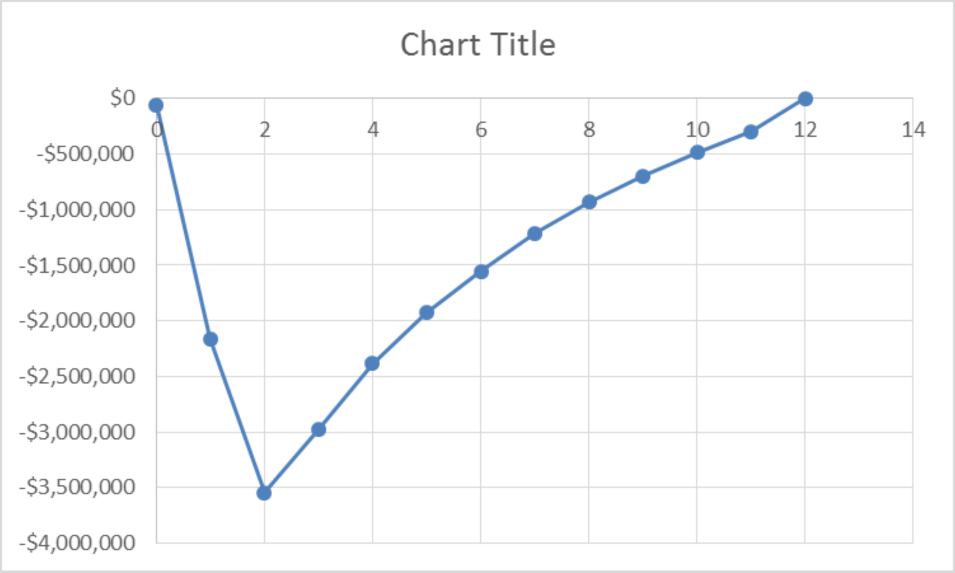
Cash Flows for a New Project



Cumulative Cash Flow Diagram

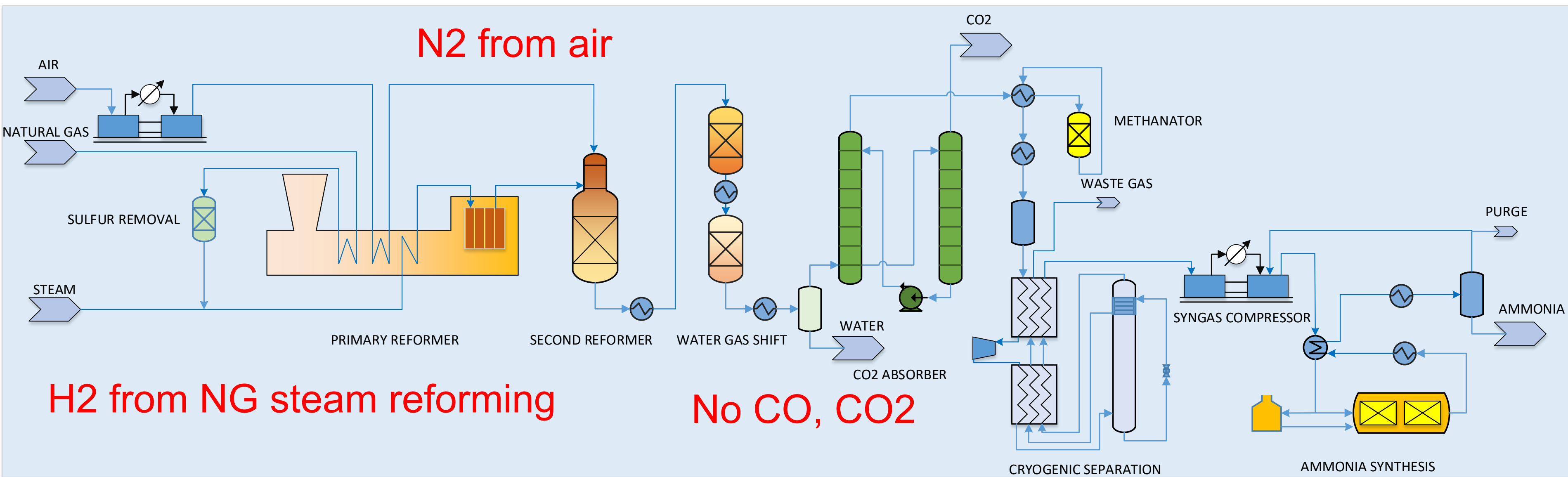
Comparison & Discussion

- Breakeven ammonia price
  - Adjust the ammonia price to have zero NPV (net present value) at the end of 12 years.
  - Breakeven to investment with 10% interest rate
- Technology Comparison
  - Traditional Haber-Bosch technology
  - Large-scale centralized water electrolysis
  - Distributed wind-based water electrolysis



Traditional Haber-Bosch Technology

- Primary steam reformer
- Secondary steam reformer
- Water gas shift
- CO_2 removal
- Methanation
- Syngas compressing
- NH_3 synthesis
- NH_3 separation

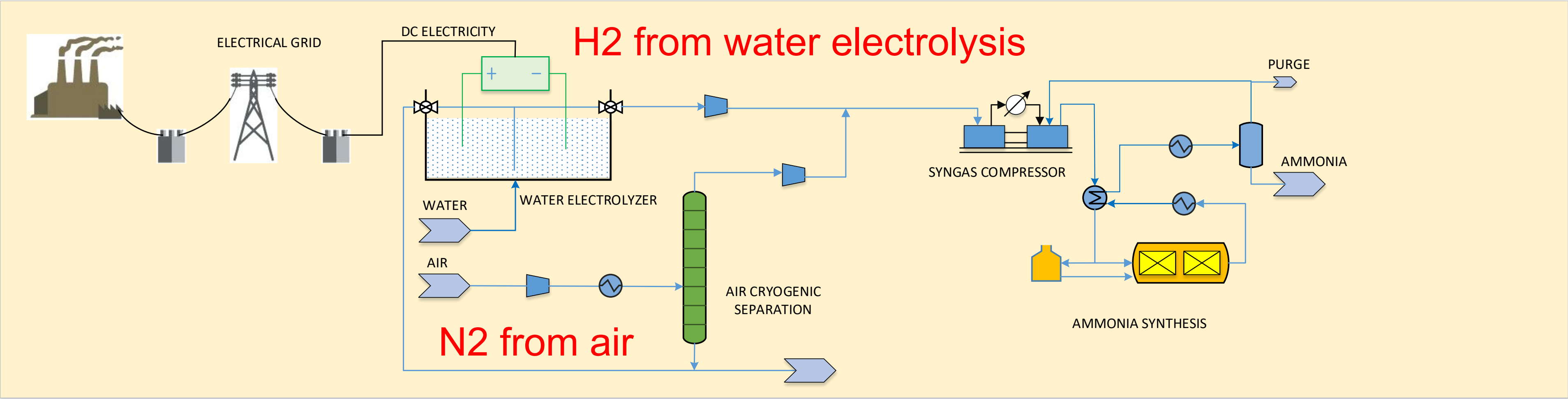


Traditional Haber–Bosch Ammonia Synthesis

In the U. S., about 98 percent of synthetic ammonia is produced by catalytic steam reforming of natural gas (70% globally).

Large-Scale Water Electrolysis

- Hydrogen comes from the large-scale water alkaline electrolysis
- Nitrogen comes from air cryogenic separation
- CO_2 emission depends on the electricity sources
- Electricity is from the grid
- Oxygen is a by-product with credit

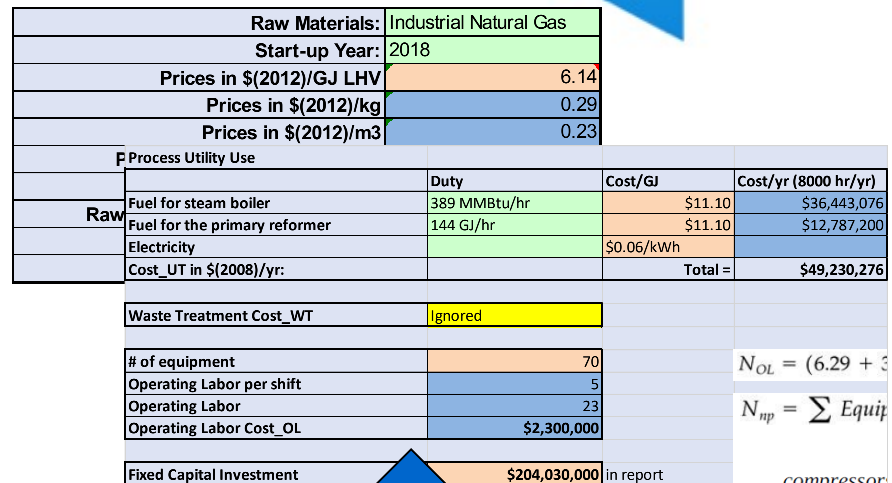


Large Scale Water Electrolysis for Ammonia Synthesis

The largest such plant in North America was a 75 MW water electrolysis/ammonia plant (200 tonne/day) at Trail, British Columbia.
Norway has 440,000 tonne/year capacity (1400t/d).

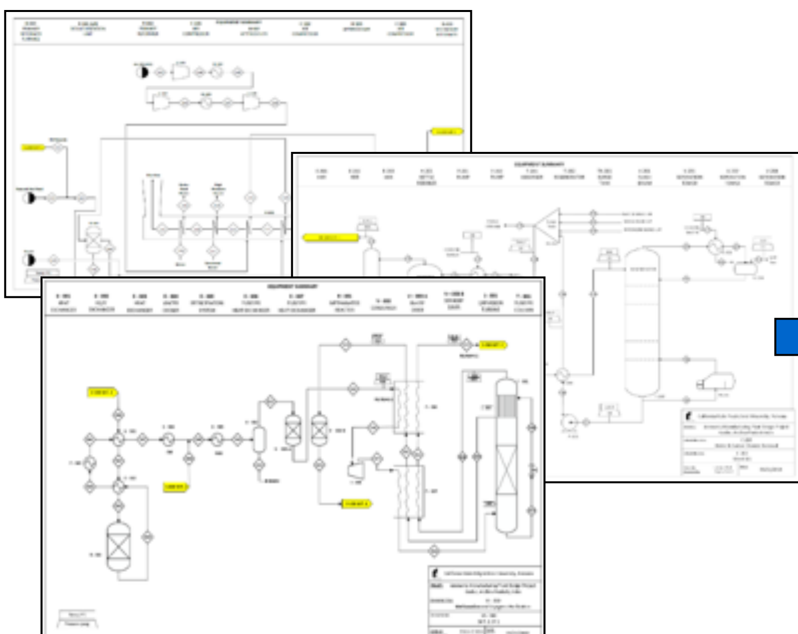
Design & Evaluation Procedure

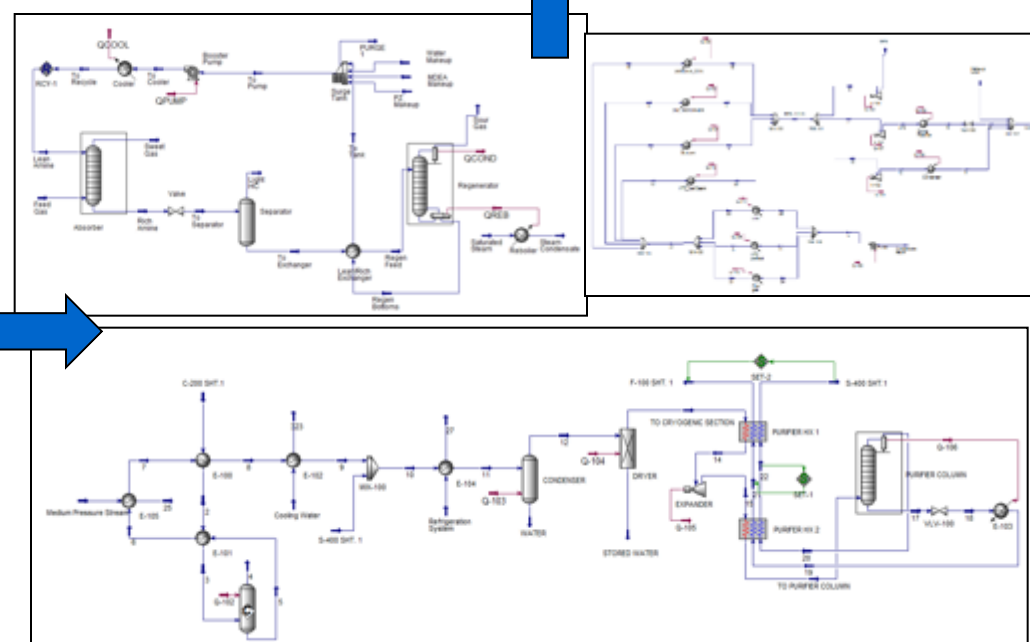
- PFDs development
- Simulation on HYSYS
- Excel-based evaluation platform
  - Equipment sizing
  - Capital cost estimation
  - Cost of manufacturing
  - Financial analysis



Raw Materials:	Industrial Natural Gas
Start-up Year:	2018
Prices in $(2012)/GJ LHV	6.14
Prices in $(2012)/kg	0.29
Prices in $(2012)/m3	0.23

Process Utility Use			
	Duty	Cost/GJ	Cost/yr (8000 hr/yr)
Fuel for steam boiler	389 MMBtu/hr	$11.10	$36,443,076
Fuel for the primary reformer	144 GJ/hr	$11.10	$12,787,200
Electricity		$0.06/kWh	
Cost_UT in $(2008)/yr:		Total =	$49,230,276
Waste Treatment Cost_WT	Ignored		
# of equipment	70		
Operating Labor per shift	5		
Operating Labor	23		
Operating Labor Cost_OL	$2,300,000		
Fixed Capital Investment	$204,030,000	in report	





Results & Comparison

- Traditional Techno-Economic Assessment (TEA) results

Items	HB	Cent. EL	Dist. EL
FCI (MM$)	214	299	850
COM (MM$/y)	205	358	543
Price ($/tNH3)	495	832	1406

- It explains why the HB technology is dominant in the existing ammonia synthesis business.
- The water electrolysis based technology is less than 1%.
- It seems there is no way for the novel distributed technology to compete with the traditional ones. However…

Results & Comparison

- However, if more evaluation areas are integrated into the evaluation system, it would highlight the advantages and show the promising development directions.
- MOMT evaluation framework results

Items	Price Change ($/tNH3)
CO2 credit ($30/tCO2)	-69
CO2 credit ($50/tCO2)	-116
Electricity 20% discount	-109
Electricity 50% discount	-273
Modular FCI 20% discount	-123
Modular FCI 50% discount	-306
Low Pressure Reactor	-154
O2 credit ($20/tO2)	-35

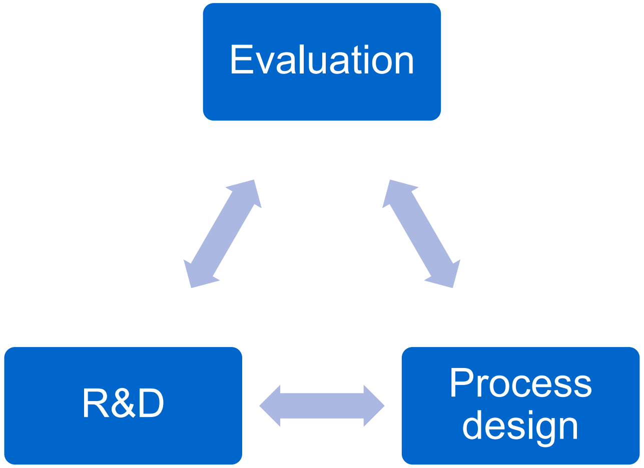
Results & Comparison

- If the developed distributed plants achieved all the potentials, the MOMT evaluation cost is $563 per tonne ammonia
- Comparable to the traditional Haber–Bosch process
- Therefore, the wind-based distributed technology is a competitive and promising technology.

Items	HB	Cent. EL	Dist. EL	*Dist.EL MOMT*
FCI (MM$)	214	299	850	*301*
COM (MM$/y)	205	358	543	*298*
Price ($/tNH3)	495	832	1406	***563***

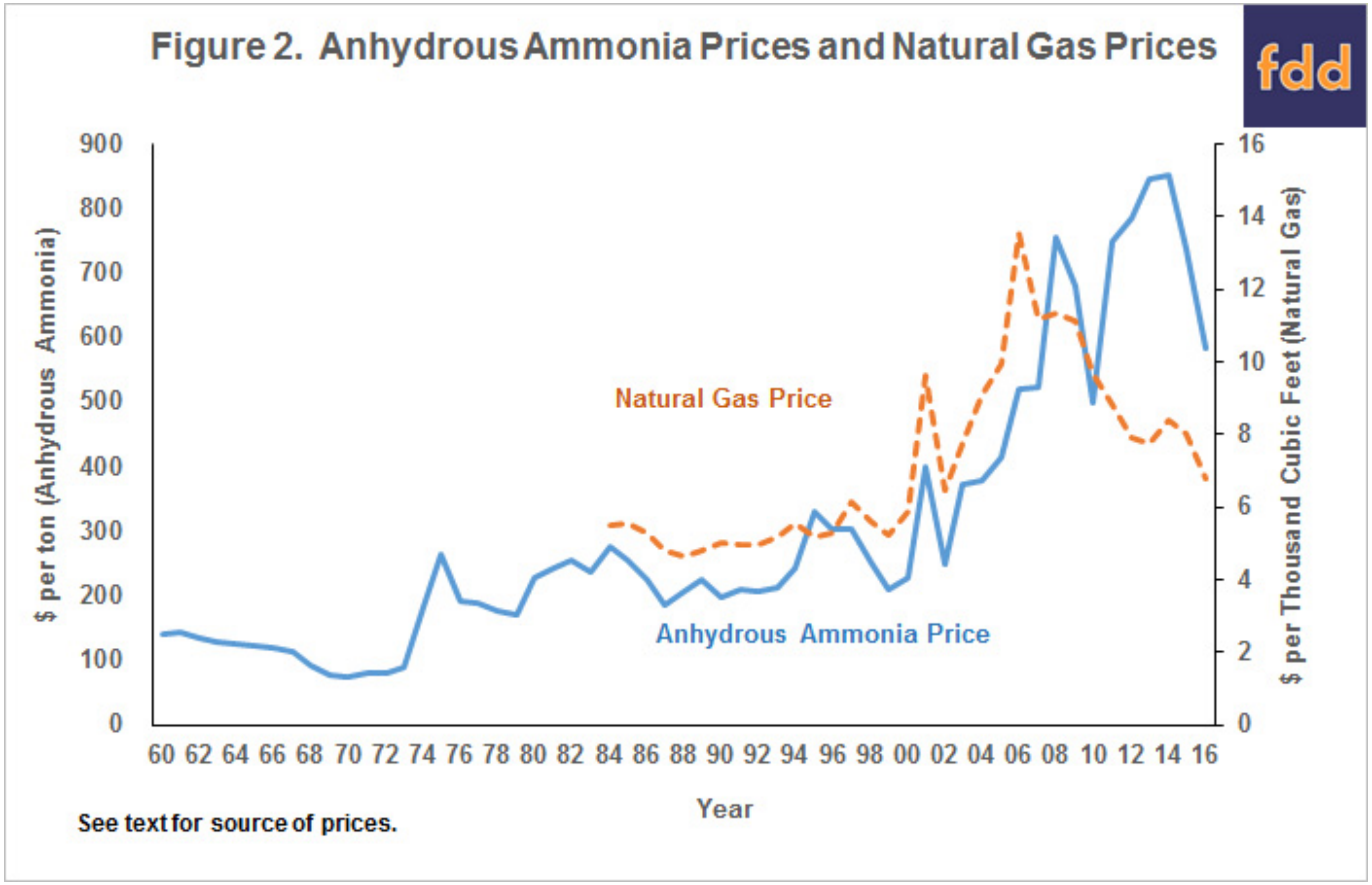
SUMMARY

- Challenges in process design and evaluation of the features in new emerging process technologies
- Multi-Objective Multi-Technology (MOMT) design & evaluation for distributed wind-based water electrolysis for ammonia synthesis
- Results & Comparison
  - The wind-based distributed technology is a competitive and promising technology
- Future Work – cooperation & more in-depth design



THANK YOU!

Q&A



https://farmdocdaily.illinois.edu/2016/06/anhydrous-ammonia-corn-and-natural-gas-prices.html

Manufacturing Cost Estimation

- Raw material cost
  - Natural gas price (location, time)
  - Electricity price (location, time, grid, wind, solar, hydropower)
- Utility cost
  - Price from typical data or from the fuel cost vis the steam and refrigeration system simulations
  - Utility use from plant-wide simulation
- Others
  - Waste treatment, labor, maintenance, etc.

Raw Materials:	Industrial Natural Gas
Start-up Year:	2018
Prices in $(2012)/GJ LHV	6.14
Prices in $(2012)/kg	0.29
Prices in $(2012)/m3	0.23
Prices in $(2012)/thousand ft3	6.41
Feed flow (kg/hr)	35655
Raw Materials Cost in $(2012)/hr:	$10,318
Operating hours per year:	8000
Cost_RM in $(2012)/yr:	$82,543,631

Process Utility Use			
	Duty	Cost/GJ	Cost/yr (8000 hr/yr)
Fuel for steam boiler	389 MMBtu/hr	$11.10	$36,443,076
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Operating Labor	23		
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Fixed Capital Investment	$204,030,000	in report	

$N_{OL} = (6.29 + 3$

$N_{np} = \sum Equip$

compressor

Emission

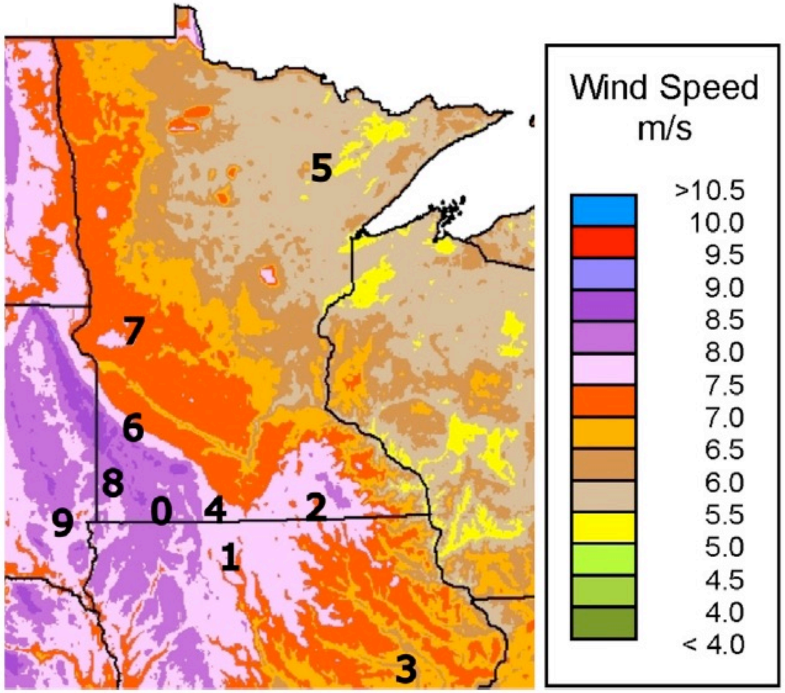
- Greenhouse Gas Emissions for natural gas, electricity, and CO_2 generation in process
- GREET: full life-cycle model sponsored by the Argonne National Laboratory.
- Multiple objectives integration
  - With adjustable weights
  - Carbon tax or credit

Central Water Electrolysis for Ammonia Synthesis Emission Analysis

Emission Items	Flow (kg/hr)	Flow (kmol/hr)	Flow (GJ/hr) LHV	Flow (GJ/kg NH3)	Upstream GHG (CO2 eq) Emission (kg/kg NH3)	Process GHG (CO2 eq) Emission (kg/kg NH3)
Natural Gas in Feed			0.0	0.00000	0.000	0.000
Natural Gas in Utility			0.0	0.00000	0.000	0.000
	Power (MW)		Power (GJ/hr)	Power (GJ/kg NH3)		
Electricity for Electrolyzer	461.3		1660.7	0.02657	5.013	0.000
Electricity for compressor	48.8		175.7	0.00281	0.530	0.000
** to be added **						
Total GHG (CO2 eq) Emission (kg/kg NH3)	5.543					
Total GHG (CO2 eq) Emission (tonne/yr)	2,771,581					

Logistics

- Distributed process development
  - Effects of location
  - Effects of plant scale
  - Effects of wind capacity
  - Effects of modular design and manufacture
- Ammonia as hydrogen/energy carrier
  - Storage and transport in liquid.
- Link to multi-objective evaluation



Allman, A., Daoutidis, P., Optimal scheduling for wind-powered ammonia generation: Effects of key design parameters. Chem. Eng. Res. Des. (2017)

Manufacturing Costs Estimation

- COM = function(RM, UT, WT, OL, FCI)
  - RM = raw materials, WT = waste treatment, UT = utilities, OL = operating labor, FCI = fixed capital investment (total module or grass roots)
- Maintenance and Repairs
  - 2 – 10 % FCI
  - Proportional to Size of Plant
- Supervisory and Clerical Labor
  - 10 – 25 % COL
  - Proportional to Operating Labor
- R&D
  - 5% of COM

FUTURE WORK

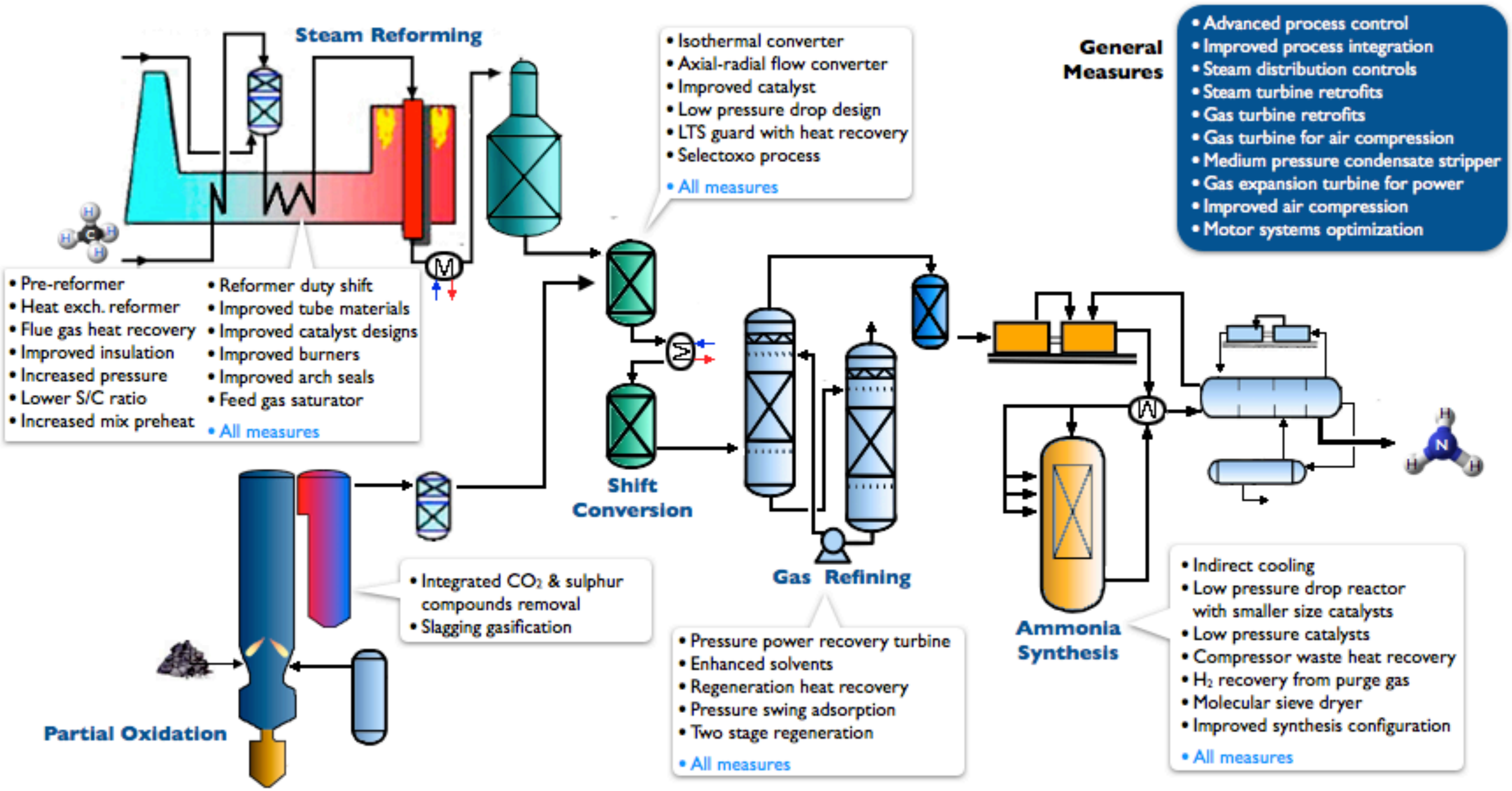
- Cost Estimation Adjustment
  - Refer to the industrial data (e.g. H-B process as benchmark)
- Continue to integrate multi-objective evaluation models
  - Waste treatment / toxics in environment
  - Logistics, scheduling, and transportation
  - Social impacts
  - Highlight merits for the distributed technology
- More in-depth study on the distributed process to provide optimal design

CAL POLY POMONA

PROCESS DESIGN EDUCATION

- Capstone process design series for the senior undergraduate students
- Extend the scope to the new emerging technologies such as biomass related process, solar or wind-based energy use, distributed modular plant, etc.
- Bridge the gap between the fundamental research to the industrial process development

- General introduction



http://ietd.iipnetwork.org/content/ammonia#technology-resources

MOMT DEVELOPMENT PROCEDURE

- Step 1: The proposed framework streamlines the classic process design layers in terms of chemistry, reaction, separation, heat exchanger network, utilities, etc. Process flow diagrams (PFDs) are developed for each process to be evaluated.
- Step 2: Process simulation is implemented of each process to provide mass & energy balance data which characterize the process performances quantitatively.
- Step 3.1: Estimate the capital cost (e.g. equipment, land, indirect, contingency cost, etc.) by sizing the process equipment and cost estimation models.
- Step 3.2: Estimate the cost of manufacturing in terms of raw materials, utilities, waste treatment, operating labor, and other capital investment related costs.
- Step 3.3: Perform financial analysis with market information to evaluate the profitability objective.

MOMT DEVELOPMENT PROCEDURE

- Step 4: According to the raw materials, side products, waste generation, utility use, etc., estimate the environmental objective related factors such as greenhouse gas emissions, waste treatment, life cycle analysis, etc.
- Step 5: For the distributed processes with biomass or wind/solar-based electricity, perform logistic analysis to estimate the transportation and scheduling.
- Step 6: Based on the multi-objective information, the processes could be evaluated and analyzed in terms of multi-objective evaluation, key parameter sensitivity study, and optimal process design. In such way, various process technologies could be compared on a consistent platform with multiple objectives.

PROCESS CONDITIONS

- Reactor conditions
  - High pressure (150 – 330 atm)
  - Temperature: tradeoff between reaction rate and equilibrium (350 – 550 C)
- Typical one-pass conversion only 25 – 35%
  - Separate NH_3 from unreacted H_2 and N_2
  - High recycle gas flow
- Feed preparation
  - N_2 from air
  - H_2 from steam reforming or water electrolysis
  - No CO, CO_2 for catalyst poison issue
  - Low inert gas for high recycle gas flow
  - H_2:N_2 = 3:1