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Technoeconomic Analysis on an Electrochemical Nonoxidative Deprotonation Process for Ethylene Production from Ethane

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EXECUTIVE SUMMARY

This report has been prepared as part of a study for Light Water Reactor Sustainability (LWRS) program to evaluate the technical and economic feasibility of integrating a light-water reactor (LWR) nuclear power plant (NPP) with an electrochemical, nonoxidative deprotonation (ENDP) process for production of ethylene from ethane. Process synthesis and modeling were utilized to assess the economic feasibility.

ENDP is a novel, early Technical Readiness Level (TRL) ~1–2 process for producing ethylene and hydrogen via the electrochemical dehydrogenation of ethane. It is currently being demonstrated at the laboratory scale at Idaho National Laboratory (INL) (Ding et al. 2018). Ethane is a plentiful feedstock that is separated as a condensate during natural-gas processing.

The U.S. LWR NPP fleet is facing increasing financial challenges due to the expansion of solar and wind power, as well as the low price of natural gas. Alternative strategies are being sought to increase the revenues of NPPs and to find new applications for NPP heat and electricity during periods of overgeneration. NPPs enable solar and wind generating-capacity buildout by providing carbon-free baseload capacity needed for times when solar and wind are unable to generate. Overgeneration occurs during periods when excess electricity is generated due to high solar- or wind-energy output. During these times, NPPs are either paying to curtail wind and solar power or are flexibly operating by turning down their reactor power and generation output. Flexible operations can have impacts on NPP fuel cycles and maintenance while also decreasing revenue. An NPP could alternatively provide carbon-free energy for process-heat steam, cooling water for cooling duties, and house-load electricity to industrial processes, such as ENDP, as an alternative revenue-generating source. In conventional chemical processes, energy and utilities are generated by utilizing fossil fuels, such as coal, fuel oils, and natural gas, resulting in significant emissions of carbon dioxide greenhouse gases (GHGs).

Ethylene production via the current industry-standard process of steam cracking, for example, is energy intensive and uses large furnaces burning large amounts of natural gas to “crack” feedstocks from ethane and naphtha to heavy gasoils into lighter olefinic molecules (such as ethylene, propylene, etc). Steam cracking is a mature and optimized industrial process, but remains both capital and energy intensive. Thus, the steam-cracking process is the subject of frequent process-intensification studies to reduce the process-energy demand (Gao et al. 2019).

The primary purpose of this report is to present a scaled modeling and technoeconomic analysis (TEA) of the novel ENDP process for producing ethylene and hydrogen from ethane. This TEA provides the related chemical process and economic analysis for the production of ethylene and hydrogen via the ENDP process and compares it with conventional industrial steam cracking of ethane for ethylene production. The modeled ENDP process is coupled with a 1000 MW hypothetical NPP, which provides low-pressure steam (275°C), standard cooling water, and electricity needed for the electrochemical process as well as resistive heating at marking prices.

Given that the ENDP process is still in the early research stage, two ENDP cases are evaluated in this study: the *projected current* (Case 1) and the predicted future (Case 2). Case 1 is based on current results obtained from laboratory results on button cells. Case 2 is a predicted future case assuming improvements to the ENDP process are made. Specific areas targeted for improvement and research which have the potential to bring about the performance improvements assumed in the future Case 2 are discussed in Section 2.5. The main difference between the two ENDP cases is the single-pass ethylene yield. The yield is 25.7% in the current case versus 48.5% in the future case at 550°C. The ENDP future predicted case assumes that technological improvements including catalyst selectivity, reactor design and system performance will be made in order to achieve the projected ethylene single pass yield. The chosen ethylene yield of 48.5% for the ENDP future case is according to data of a steam-cracking reference process (Thiruvenkataswamy 2015). Both ENDP cases were modeled in AspenPlus according to the conversions and yield percentages obtained from lab data for Case 1 and projected for Case 2. The feed rate of ethane in the model was scaled to match the reference industrial-scale steam-cracking process. The technical results from both cases are compared with those of a reference conventional steam-cracking process. And the economic results from the ENDP Case 2 is compared to those of the steam cracking. The cases investigated in this report are summarized in Table ES-1.

Table ES-1. Cases analyzed in this study.

	ENDP current Case 1	**ENDP future Case 2**	**Steam Cracking**
Ethane feed, tpa (kg/hr)	0.98 million tpa (111,000 kg/hr)		
Single-pass ethylene yield, %	25.7	48.5	52.4
Reactor operating temperature, ℃	550	550	850

Figure ES-1 shows the overall energy and mass balance for the ENDP future predicted case integrated with a 1000 MW_e NPP. For an ethane feed of 111 metric tons (tonne) per hour, the ENDP plant produces 84 tonne/hour ethylene, 7 tonne/hour of hydrogen, and a stream of 20 tonne/hour of other C_3 to C_4 hydrocarbons, which can be sold as a coproduct stream. This process requires 420 MW_e power, 140 MW_t steam, and 25 MW_t cooling duty from an NPP, the sale of which can provide revenue for the NPP.

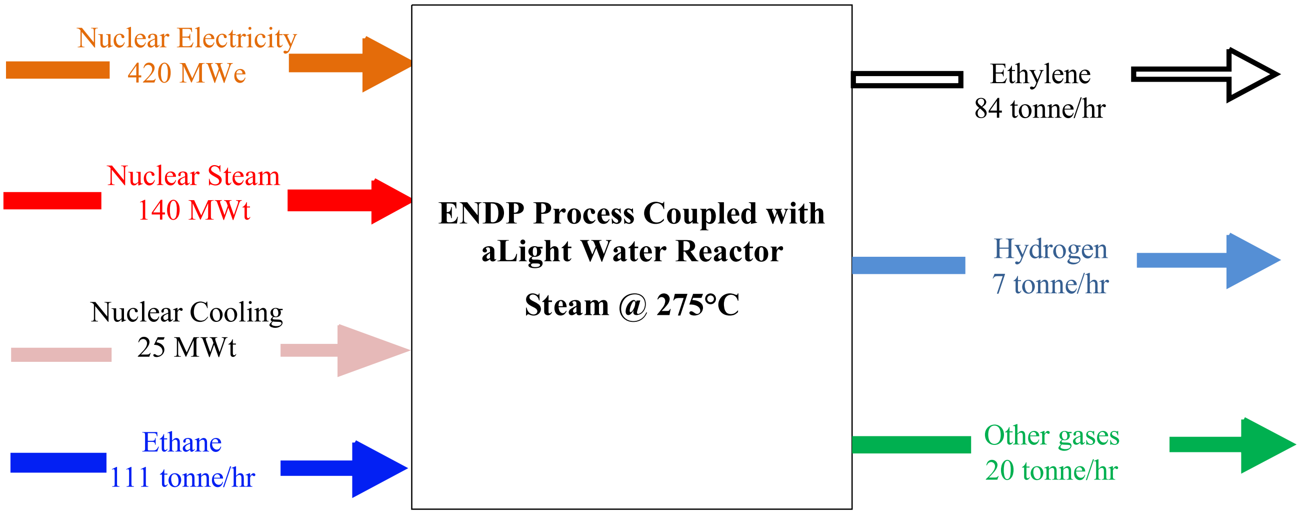

Figure ES-1. Overall energy and product flows for the LWR/ENDP integration case (electricity, steam and cooling water are purchased from a NPP).

The ENDP future case exhibits several advantages over traditional steam cracking, including a 50% reduction in capital costs (Figure ES-2), a 20% decrease in operating costs (Figure ES-3), a 77% reduction in process energy required, and a more than 70% reduction in carbon footprint.

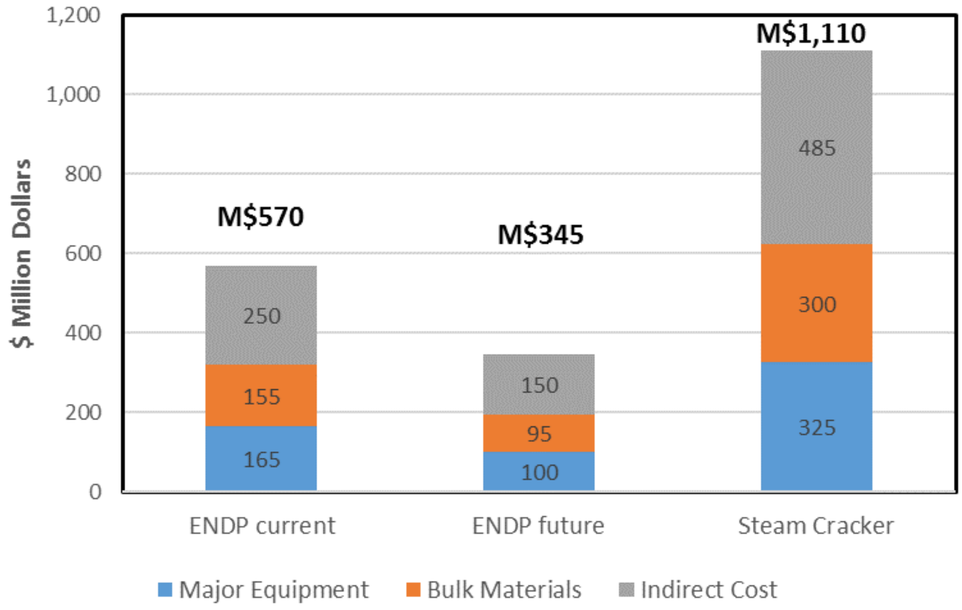

Figure ES-2. Comparison of capital costs for the ENDP and steam-ethane cracking.

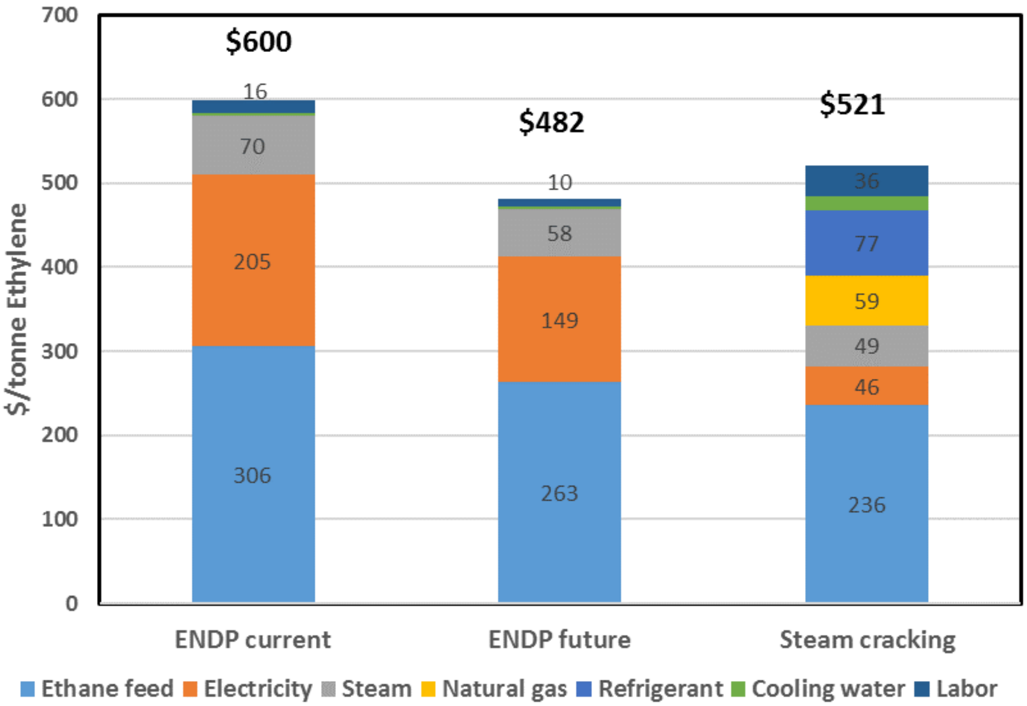

Figure ES-3. Comparison of relative direct operating costs for ENDP and steam-ethane cracking.

For the ENDP future case with an internal rate of return (IRR) of 12% and a selling price for ethylene at $0.44/kg ($0.2/lb), the anticipated net present value (NPV) for this project is $285M and the discounted payback period is five years of operation (Figure ES-4). It is worth noting that the current industrial ethylene selling price is near $0.44/kg ($0.2/lbs) which is, historically, a record low price (HIS 2019). When the NPV is set equal to zero at an IRR of 12%, the minimum selling price (MSP) of ethylene is $0.37/kg for Case 2. This MSP is the price at which the project will break even, which is 48% lower than that of steam cracking ($0.71/kg), indicating a promising economic feasibility when compared to the conventional steam-cracking process. The high MSP of the steam-cracking process is mainly due to its high capital costs ($1,110M), which are more than three times higher than that of the ENDP future case.

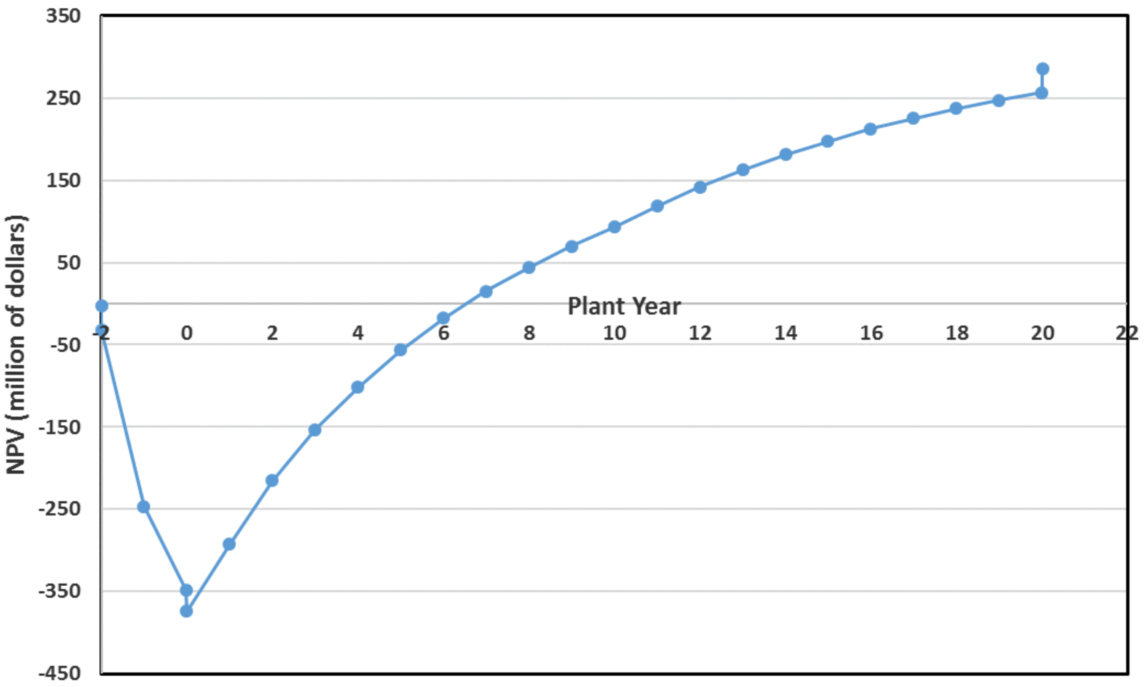

Figure ES-4. Discounted cash-flow diagram for the ENDP future case at IRR 12% and $0.44/kg of ethylene.

Sensitivity analysis was conducted on factors affecting the MSP of ethylene for the ENDP future predicted case (Figure ES-5). At the base value of each factor, the MSP is calculated as $0.37/kg ethylene produced. Figure ES-5 demonstrates the percentage change versus the baseline price by varying each factor from low to high range, which are based on historical data. The price of feed ethane is the biggest influencer, causing 35% variation on the MSP of produced ethylene for every $0.1/kg change of ethane, followed by the prices of electricity, hydrogen and propylene.

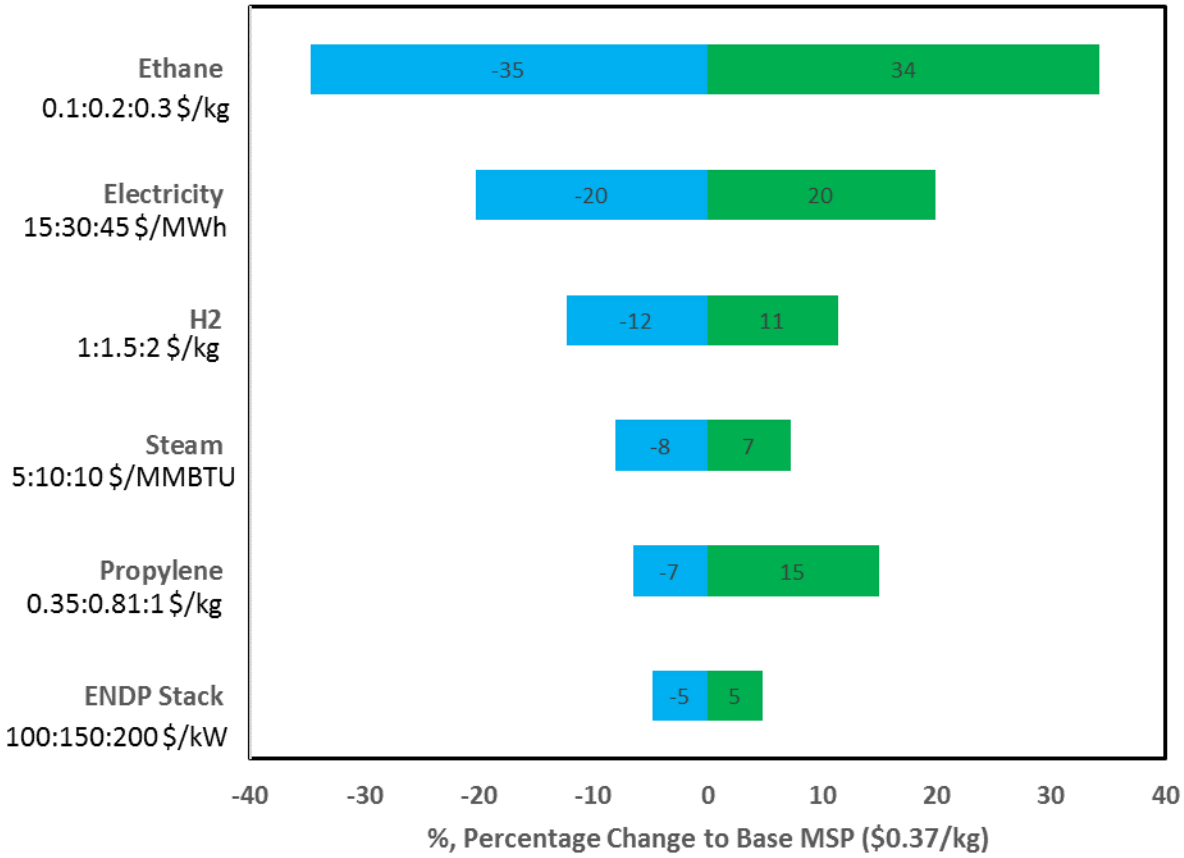

Figure ES-5. Sensitivity analysis on factors affecting the MSP of ethylene for ENDP future case 2

Overall, integration of nuclear heat and power into an ENDP process for ethylene production appears promising when compared to the conventional steam cracking process for producing ethylene. Analysis shows that scaling of the ENDP process from the lab to the plant could be economically feasible. The MSP of ethylene is lower than the current average market price in the United States. Additionally, life-cycle carbon emissions could be significantly reduced by employing the ENDP process versus the conventional steam cracking process.

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FIGURES

TABLES

ACRONYMS

AAGR	average annual growth rate
APEA	Aspen Process Economic Analyzer
ASR	area-specific resistance
ATCF	after-tax cash flow
BOP	balance of plant
BTCF	before tax cash flow
BWR	boiling-water reactor
CAPEX	capital expenditures
CMS	compact membrane systems
COP	coefficient of performance
DCC	direct capital cost
DCFROR	discounted cash-flow rate of return
DOE	Department of Energy
DPBP	discounted payback period
ENDP	electrochemical nonoxidative deprotonation
EUCG	Electric Utility Cost Group
GHG	greenhouse gases
HDPE	high-density polyethylene
HHV	higher heating value
HTE	high-temperature (steam) electrolysis
HTSE	high-temperature steam electrolysis
INL	Idaho National Laboratory
IRR	internal rate of return
JT	Joule-Thomson (valve)
LHV	lower heating value
LDPE	low-density polyethylene
LLDPE	linear low-density polyethylene
LPG	liquified petroleum gases
LWR	light-water reactor
LWRS	Light Water Reactor Sustainability
MACRS	modified accelerated cost recovery system
MR	mixed refrigerant
MSP	minimum selling price

mtpa	million tonnes per annum
NG	natural gas
NHES	nuclear-renewable hybrid energy system
NPP	nuclear power plant
NPV	net present value
NREL	National Renewable Energy LaboratoryO&M operating and maintenance
OCF	operating-capacity factor
ODH	oxydehydrogenation
OPEX	operating expenses
OSTG	once-through steam generators
PBSCF	PrBa0.5Sr0.5Co1.5Fe0.5O5+d
PE	polyethylene
PEM	polymer-electrolyte membrane
PFD	process-flow diagram
PP	polypropylene
PSA	pressure swing adsorption
PWR	pressurized water reactor
SEC	specific-energy consumption
SEM	scanning electron microscopy
SOEC	solid-oxide electrolytic cells
TCI	total capital investment
TEA	technoeconomic assessment
tpd	tonnes per day
TRL	technology readiness level

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Technoeconomic Analysis on an Electrochemical Nonoxidative Deprotonation Process for Ethylene Production from Ethane

1. INTRODUCTION

This report has been prepared as part of a study for the Light Water Reactor Sustainability (LWRS) program to evaluate the technical and economic feasibility of scaling a new electrochemical nonoxidative deprotonation (ENDP) process from the laboratory measurement to plant scale and of integrating nuclear-power-plant (NPP) steam and electricity with the ENDP process for production of ethylene and hydrogen from ethane. Process synthesis and modeling were utilized to assess technical and economic feasibility.

Currently, a total of 57 NPPs operate a total of 96 nuclear reactors in United States; these operations provide 20% of America's total electricity and contribute nearly 60% of overall carbon-free energy. Their average generating costs have decreased from a peak of $40.25/MWh in 2012 to $33.93/MWh in 2016 (EUCG 2017) and continue to decrease below $30/MWh as nuclear plant operators continue to drive costs down to stay competitive. However, the current NPP fleet still faces financial challenges. The revenue gap is the difference between electricity-market revenue earned by a nuclear unit located in a wholesale electricity market and the generating costs of that nuclear unit. Analysis of the revenue gap over 79 of 98 then operating NPPs revealed that 80% (63 out of 79) of the units analyzed had a negative revenue gap (EUCG 2017). This is mainly due to electricity-market conditions, which result in low electricity prices because:

- Markets are not structured to recognize the valuable attributes of different energy sources, like GHG and other emissions avoidance, reliability, resiliency, and onsite fuel burn time
- Energy companies price their electricity based on short-term costs, making long-term investments difficult to afford
- Solar and wind generating capacity continues to expand
- Natural-gas prices are persistently low.

Alternative strategies are being sought to increase the revenues of NPPs and to find new applications for NPP heat and electricity during periods of overgeneration that produce negative operating margins for NPPs. NPPs enable solar and wind generating-capacity buildout by providing carbon-free baseload capacity needed for times when solar and wind are unable to generate. Overgeneration occurs during periods when excess electricity is generated due to high solar- or wind-energy output. During these times, NPPs either pay to curtail wind and solar power or operate flexibly, turning down their reactor power and generation output. Flexible operations negatively impact NPP fuel cycles and maintenance while also decreasing revenue.

An NPP could, alternatively, provide carbon-free energy for process-heat steam, cooling water for cooling duties, and house-load electricity to industrial processes, such as ENDP, as an alternative revenue-generating source. In conventional chemical processes, energy and utilities are generated by utilizing fossil fuels such as coal and natural gas, resulting in significant emissions of carbon dioxide GHGs. Additionally, it is possible that the receiving industrial process, such as ENDP, can benefit economically from low-priced house-load nuclear electricity during periods of overgeneration when NPP operating margins would otherwise be negative.

Ethylene production via the current industry-standard process of steam cracking, for example, is energy intensive and uses large furnaces burning large amounts of natural gas to "crack" feedstocks from ethane and naphtha to heavy gasoils into lighter olefinic molecules. Steam cracking is a mature and optimized industrial process, but remains capital and energy intensive. Thus, the steam-cracking process is the subject of frequent process-intensification studies to reduce the process-energy demand (Gao et al., 2019).

The primary purpose of this report is to present a scaled modeling and technoeconomic analysis (TEA) for a novel ENDP process for producing ethylene and hydrogen from ethane. Additionally, this report describes how nuclear-generated heat and electricity could be integrated into the ENDP process synergistically, allowing both the ENDP process and the NPP operations to be more economical. This TEA provides the related economic analysis for the production of ethylene and hydrogen via the ENDP process and compares it with conventional industrial steam cracking of ethane for ethylene production.

The ENDP process was scaled from laboratory to plant scale using chemical-process simulation software (AspenPlus). This report assumes familiarity with AspenPlus; hence, a detailed explanation of the software capabilities, thermodynamic packages, unit-operation models, and solver routines is beyond the scope of this report. Similarly, a familiarity with steam cracking, electrochemical processes, and common purification and separations technologies is assumed.

The structure of this report includes an overview of the process-modeling methodology and results for various case studies. Next, an overview of the economic-modeling methodology and results is presented. Emphasis is placed on the feasibility of the new ENDP process upscaling and the impact of the NPP integration. Finally, overall conclusions for the ENDP process compared to the steam cracking process are discussed.

1.1 Ethylene Production Methods and Market Overview

1.1.1 The Ethylene Market

Ethylene is one of the most important building blocks for the petrochemical industry and is among the most produced organic compounds (Emerson 2010). Ethylene is used as a feedstock for various polymers and derivatives, such as polyethylene, ethylene dichloride, ethylene oxide, ethylene glycol, ethyl benzene, vinyl acetate and other miscellaneous chemicals. These chemicals are then used for the production of end products, including food packaging, film, toys, food containers, bottles, pipes, antifreeze, carpets, insulation, housewares, etc. (Emerson 2010).

Global ethylene capacity is projected to see 27% growth, from 207.58 million tonnes per annum (mtpa) in 2019 to 264.13 mtpa in 2023 (GlobalData 2019). Around 126 planned and announced ethylene plants are scheduled to come online, predominantly in Asia and North America, over the next four years, as shown in Figure 1 (GlobalData 2019).

North America is the second highest region in terms of capacity addition in the global ethylene industry, growing at an average annual growth rate (AAGR) of 4.1% from 53.60 mtpa in 2019 to 63.22 mtpa in 2023. Most ethylene capacity additions will be from the U.S., with a capacity of around 14.55 mtpa by 2023. Major capacity additions will be at the Exxon Mobil Corporation Baytown Ethylene Plant 1, with a capacity of 2.30 mtpa by 2023. In North America, the low-cost abundant supply of shale natural gas is the primary reason for the rise in ethylene capacity additions in the U.S.

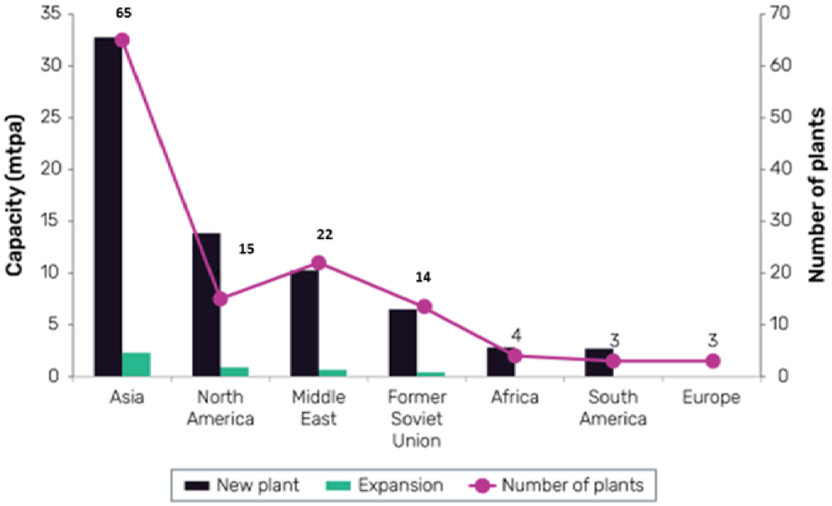

Figure 1. Global planned and announced ethylene capacity additions by key regions (in mtpa) by 2023. [Source: GlobalData 2019]

1.2 Ethylene Production from Steam Cracking

The predominant industrial process for ethylene production is thermal cracking of ethane and naphtha feedstocks in the presence of steam, which is also known as steam cracking or thermal pyrolysis. Natural-gas condensate feeds (ethane, propane, and n-butane) accounted for nearly 90% of the fresh feed for U.S. ethylene plants in 2015 due to the increased shale-gas production since 2009 (Thiruvenkataswamy 2015).

Literature studies also reveal that specific consumption of ethane is much higher than that of naphtha (Ren et al. 2006). Other advantages of using ethane feedstock are low CO_2 emissions, high ethylene and hydrogen yield, and fewer heavy products to manage (Ren et al. 2006). Table 1 illustrates the comparison of different steam-cracker feedstocks. Oil-based petrochemical feedstocks such as naphtha and gasoil, have only modest yields of ethylene (around 25–30%) whereas lighter liquified petroleum gases (LPGs) and gas-associated hydrocarbon compounds, such as ethane, have significantly higher ethylene yields when cracked (up to ~80%). As a result, a smaller volume of feedstock input is required to yield ethylene from ethane and LPGs than from oil-based naphtha and gasoil, significantly influencing petrochemical plant economics. According to industry analysts, it takes just 1.302 tonnes of ethane to yield 1 ton of ethylene, compared with some 3.3 tonnes of naphtha input for the same result (Brooks 2013).

Three main process sections are usually involved for steam cracking: cracking, compression and drying, and separation. Although steam cracking is the industry standard for ethylene production, it has disadvantages. This process is non-catalytic and non-selective and is extremely energy and capital intensive, yielding many byproducts that require extensive separations and purification (Maffia et al. 2016, Gaffney and Mason 2017). It represents the single most energy-consuming process in the chemical industry. Ethane steam cracking consumes typically 17–21 GJ specific-energy consumption (SEC) of process energy per ton of ethylene (Ren et al. 2006), of which 65% is used in high-temperature pyrolysis, 15% in fractionation and compression, and 20% in product separation. It is estimated that the steam-cracking process comprises60% of the ethylene-product cost and two-thirds of the manufacturing carbon footprint (Ding et al. 2018).

Either natural gas or part of the light effluent from the steam-cracking product gas stream must be combusted to provide heat for the furnaces, thereby leading to the formation of CO_2 and NO_x. Per ton of ethylene, 1–1.6 t of CO_2 are produced through this external heating (Gartner et al. 2013). In addition, notable amounts of coke are formed on the inside furnace-tube walls, requiring regular furnace shutdowns for maintenance and coke removal by air and steam gasification (Gartner et al. 2013) because mechanical coke removal is not possible.

Table 1. Steam-cracker yields of various petrochemical feedstocks. [Source: Fattouh and Brown 2014, Ding et al. 2018]

	Feedstock				
Yield by weight (%)	**Ethane**	**Propane**	**Butane**	**Naphtha**	**Gasoil**
H_2 and CH_4	13	28	24	26	18
Ethylene	50-80	45	37	30	25
Propylene	2	15	18	13	14
Butadiene	1	2	2	5	5
Mixed butenes	2	1	6	8	7
C_{5+}	2	9	13	8	7
Benzene	0	0	0	5	5
Toluene	0	0	0	4	3
Fuel oil	0	0	0	2	18

1.3 Ethylene Production from Catalytic Oxidative Dehydrogenation

Catalytic dehydrogenation of ethane has emerged by adopting highly selective catalysts such as Pt, Pd, or CrO_X (Gartner et al. 2013). The strongly endothermic and equilibrium-limited process is performed in fixed-bed reactors according to the following reaction:

$C_2H_6 = C_2H_4 + H_2$,
Ethane = Ethylene + Hydrogen

Thermodynamics dictate the use of high temperatures and low pressures. For instance, at atmospheric pressure, reaction temperatures of 550 and 700°C are required to reach ethane equilibrium conversions of 10 and 40%, respectively. Ethane conversion has been reported to be 15% at 600°C and not more than 40% at 650–700°C (Ding et al. 2018). This can be compensated for by operating at higher temperatures, but side reactions, coke formation, and catalyst deactivation are also accelerated. High pressure shifts the equilibrium toward ethane. Because of thermodynamic limitations, it is difficult to improve the ethane conversion.

Specifically, the major challenges are the suppression of side reactions and the formation of a suitable pellet shape of the catalysts, which ensures efficient feed distribution and minimizes pressure drop. Consecutive side reactions lead to the formation of dienes, polymers, and coke. Coke removal from the catalyst during the frequent regeneration is required to maintain acceptable catalyst lifetimes. Regular catalyst regeneration occurs by oxidation and the associated heat of combustion can be recovered in a straightforward manner, especially if several catalyst beds are operated in parallel.

To improve conversion at reduced temperatures, the catalytic oxidative dehydrogenation, or oxydehydrogenation (ODH) of ethane has been proposed (Gartner et al., 2013). In the ODH process, oxygen is added to the feed in order to burn some material to create heat for the process (Gartner et al., 2013). Its conceptual advantage over dehydrogenation, as described above, is high ethane conversion, an exothermic reaction, and potentially lower reaction temperatures required (about 300–600°C) compared to steam cracking.

$C_2H_6 = C_2H_4 + H_2$,

The conversion in the ODH process is theoretically close to unity and could bring potential energy saving of approximately 35% (Ren et al. 2006). However, new challenges are presented with this process. First, O_2 is added to the feed, thus imposing additional safety measures to prevent thermal runaway of the reaction. Second, the development of suitable catalysts is particularly challenging because olefin products tend to be more reactive than reacting alkanes, thus leading to unwanted side reactions and loss of the desired product. The relatively higher reactivity of the olefins is attributed to enhanced additional directed bonding to most catalytic surfaces, whereas alkanes interact almost exclusively through dispersion forces.

As a result, the process must be operated at low conversions in order to reach high selectivity (Gartner 2013). This seems to be a paradox unless highly selective catalysts can be discovered. Moreover, the relatively low energy efficiency, higher CO_2 emission, and additional process-safety considerations are major challenges (Ren et al. 2006).

1.4 Ethylene Production from Electrochemical Nonoxidative Deprotonation

In order to fully exploit the potential of ethane as a feedstock, it is vital to develop new disruptive methods that are both low-thermal-budget and low-carbon-footprint. ENDP is one of these methods, a newly developed technology for coproduction of ethylene and hydrogen from ethane at lower temperature (i.e., 400–500°C). It has demonstrated advantages over the traditional steam-cracking process in both energy use and CO_2 emissions (Ding et al. 2018). By applying an ENDP system, the petrochemical manufacturing paradigm is shifted from widely used thermal practices to a clean-energy regime, assuming the electricity used in the ENDP process is from a carbon- and emissions-free source like nuclear energy.

The ENDP process has been demonstrated at laboratory scale by using electrolytic button cells. The electrolytic cells consist of a superior proton-conducting electrolyte thin film, a porous anode support, and a porous cathode. Figure 2(a) shows a depiction of the reaction at the molecular level. A scanning electron microscopy (SEM) image in Figure 2(b) shows the configuration and composition of an ENDP cell. Ethane is fed to the Ni-BZCYYb anode and electrochemically deprotonated into ethylene and protons when an electrical field is applied. The generated protons transfer through the dense BZCYYb proton-conducting membrane to the PrBa0.5Sr0.5Co1.5Fe0.5O5+d (PBSCF) cathode, where they combine with electrons and form high-purity hydrogen. The rate of the reaction is controlled by the kinetics of the ethane-oxidation reaction (e.g., deprotonation), and the hydrogen-evolution reaction, while the flux of protons (H+) is controlled by the applied voltage across the membrane.

The electrolyte of the ENDP cells is acceptor-doped barium zirconate cerate (BaZr0.1Ce0.7Y0.1Yb0.1O3_d, BZCYYb), which exhibits high ionic conductivity at 400°C with a small activation energy (Ding et al. 2018). In addition, this type of material has a very high proton-transfer number at temperatures lower than 550°C, allowing pure proton conduction at high flux under reduced operating temperatures, where coking is restrained thermodynamically. A fully assembled cell consisted of a dense 10 μm-thick BZCYYb electrolyte thin film on a porous BZCYYb-Ni anode support (300 μm), and a porous double perovskite PBSCF layer (30 μm) as a cathode (Figure 2[b]). Ni is an excellent catalyst for the ethane-oxidation reaction, and the PBSCF family has been demonstrated to be triple-conducting materials ($H^+/O^{2-}/e^-$) that have good activity for hydrogen-evolution reactions.

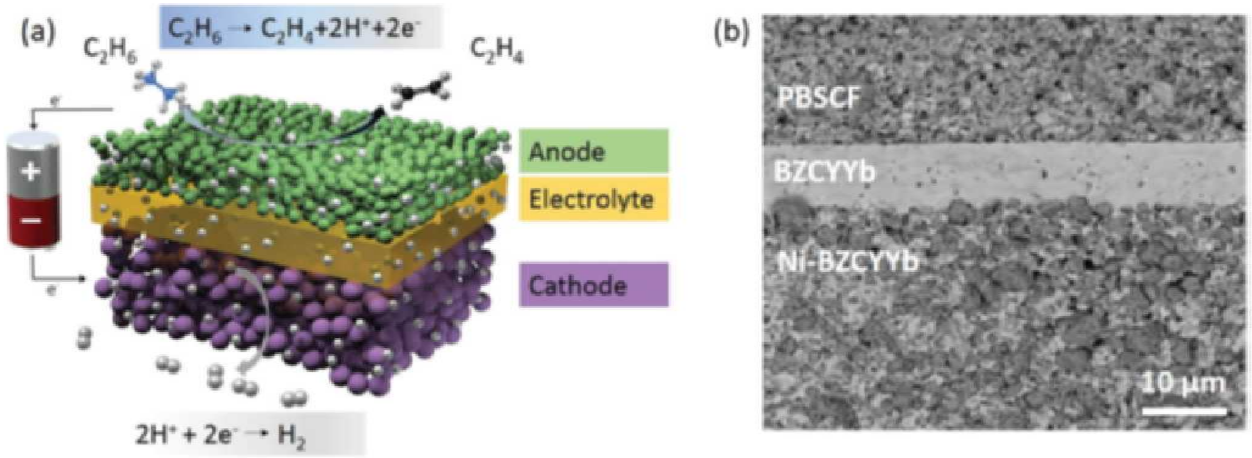

Figure 2. ENDP process and cell illustration. (a) Depiction of an ENDP cell for coproduction of ethylene at anode and hydrogen at cathode and (b) a cross-sectional SEM image of an actual ENDP cell after testing at 400°C. A porous BZCYYb-Ni anode 300 µm Ni anode (300) supported BZCYYb electrolyte (10 µm) with a porous layer of PBSCF cathode on top (30 µm). (Ding et al. 2018)

1.5 Polyethylene Production

One of the largest uses of ethylene is in the polymerization process to produce polyethylene (PE). PE is the largest-volume produced polymer worldwide, with a production of nearly 100 million metric tons, valued at $164 billion, in 2018. World demand is forecasted to be strong with compounded annual growth rate of 4% (Freedonia 2018). Polyethylene is the most widely used plastic due to its versatility, easy processability, low cost, and recyclability. Polyethylene is produced from the polymerization of ethylene, an organic chemical derived from natural gas or crude oil. Due to growth in new feedstock sources such as shale gas and biomass, PE will continue to have a price advantage over other manufactured plastics. Moreover, continually improving polymerization-catalyst technologies will enhance the performance, customization, and yield of polyethylene resins. Further increases will be limited, however, by the highly commoditized and mature position of polyethylene. Additionally, major polyethylene applications such as plastic bags, have increasingly become subject to environmental regulations and bans.

Through the polymerization of ethylene ($CH_2 = CH_2$), PE is produced with the action of initiators and catalysts (Malpass 2010). PE with various properties can be produced through different combinations of initiators, catalysts, cocatalysts, comonomers, and reaction conditions. The molecular weight of these PE varieties ranges from tens of thousands to nearly ten million amu. Among the different PEs, there are three types of PE that are widely produced across the world: low-density polyethylene (LDPE), linear low-density polyethylene (LLDPE), and high-density polyethylene (HDPE). Further manipulation of these PE varieties' properties can be achieved by the copolymerization of ethylene with other comonomers, such as short-chain alpha olefins (1-butene, 1-hexene, 1-octene), cyclic olefins, vinyl alcohol, and vinyl acetate. A wide range of catalyst are used to produce PE—for example, organic peroxides, transition-metal catalysts (Ziegler-Natta and Phillips) and single-site transition-metal catalysts (Malpass 2010).

The four principal technologies used in the production of PE are as follows (Malpass 2010):

- High-pressure tubular or autoclave
- Slurry or suspension
- Gas phase
- Solution.

High-pressure tubular or autoclave processes are used to manufacture LDPE, whereas the other three processes can be used to make LLDPE and HDPE. The four technologies operate at different pressures and temperatures. However, due to the large heat of polymerization, all processes must employ efficient heat removal. Ethylene from steam cracking can be fed directly to many of these processes with little or no purification because ethylene-product purity from the ethylene-production unit is as high as 99.95%. However, purification is usually required for processes that utilize transition-metal catalysts. Part-per-million levels of water, oxygen, CO, CO_2, acetylenics, and sulfur compounds can be damaging to those catalysts.

The production process for LDPE has been well developed for several decades (Lack 2001). LDPE is produced in a high-pressure process at temperatures in excess of 200°C and pressures from 15,000–45,000 psig. Peroxide-catalyzed polymerization takes place in either thick-walled autoclaves or tubing reactors. Ethylene purification is not necessary for the high-pressure process. Upstream of the reactor is a multistage compressor to increase pressures and temperatures to required levels. Downstream of the reactor are high-pressure and low-pressure flash vessels to isolate the polymer from excess ethylene. Unreacted ethylene is recovered and recycled to the polymerization reactor. Once isolated, the PE is pelletized. Safety is a key consideration in the production of LDPE. The two greatest hazard potentials are handling organic peroxides and the possibility of ethylene decomposition in the reactor. These risks can be mitigated through proper training and process design.

In the slurry or suspension processes, ethylene polymerization takes place in an added solvent in which polyethylene is insoluble. Added solvents are typically saturated hydrocarbons such as propane, isobutane, and hexane. Reaction temperatures range from 80 to 110°C, with pressures of 200–500 psig. Catalysts for the reaction are typically chromium supported on silica or supported Ziegler-Natta catalysts; both transition-metal catalysts. 1-Hexene is the most common comonomer used to produce LLDPE. The Chevron Phillips loop slurry process is commonly used for the production of LLDPE while the Hostalen slurry-cascade process is used to produce a wide range of molecular-weight distributions of HDPE.

Gas-phase processes operate at the same pressure and temperature ranges as slurry processes. The predominant catalysts are Ziegler-Natta. Gas-phase processes typically use a fluidized-bed reactor and are used to produce both HDPE and LLDPE.

The solution processes use either cyclohexane or C_8 aliphatic hydrocarbons as solvents. Reaction operating conditions are more severe than the slurry or the gas-phase processes, with temperatures in the 160–220°C range and pressures ranging from 500 to 5,000 psig. Polymerization takes place in the solvent where the polyethylene is maintained in the liquid phase. More recently, a combination of processes has been used in the production of LLDPE and HDPE.

2. PROCESS MODELING

2.1 Cases Considered

In this study, the ENDP process was scaled from laboratory measurements to a hypothetical plant scale and simulated using AspenPlus to obtain material and energy balances and then conduct economic analyses. The results are compared with those of a traditional reference steam-cracking process (Thiruvenkataswamy 2015). The cases analyzed in this study are list in Table 2.

Considering that the ENDP process is still in the early TRL ~1–2 research stage, two economic cases were evaluated: Case 1, a *predicted current* case based on 2019 lab-scale technology, and Case 2, a *projected future* case based on expected technology advancements by 2025. The justification for this projected increase in performance is discussed in detail in Section 2.5. Future Case 2 is hypothetical, showing performance increases that could potentially be realized if progress is made in technological and process areas mentioned in Section 2.5. The main difference between the two cases is the single-pass ethylene yield inside the ENDP reactor, which is 25.7% for the current case compared to 48.5% for the future case. The chosen ethylene yield of 48.5% for the ENDP future case is according to data of a steam-cracking reference process (Thiruvenkataswamy 2015). Both ENDP cases were modeled in AspenPlus according to the conversions and yield percentages obtained from laboratory data for Case 1 and projected for Case 2. The feed rate of ethane in the model was scaled to match the reference industrial-scale steam-cracking process.

The reference steam-cracking process has an ethylene production rate of 0.83 mtpa, which represents a medium-size steam cracker (Koottungal 2015). The corresponding ethane-feed flow rate is 0.98 mtpa . This same ethane feed rate of 0.98 mtpa (111,000 kg/hr) is used in modeling the ENDP process for comparison. The modeled ENDP process is coupled with a 1000 MW hypothetical NPP, which provides low-pressure steam (275°C), standard cooling water, and electricity needed for the electrochemical process as well as resistive heating.

Table 2. Cases analyzed in this study.

	ENDP current Case 1	**ENDP future Case 2**	**Steam Cracking**
Ethane feed	0.98 mtpa (111,000 kg/hr)		
Single-pass ethylene yield, %	25.7	48.5	52.4
Reactor operating temperature, ℃	550	550	850

A detailed description follows of the process technology, simulation techniques used, assumptions made, and results of steady-state simulation. A caveat for the economic analysis is that only major equipment involved in the main-process stream flow were considered for analyzing the process. AspenPlus, Version 10, was used to carry out steady-state simulation. Peng Robinson was used as the base thermodynamic method for simulation of both ENDP cases. All reactors were simulated using the AspenPlus RSTOIC model while all distillation columns were simulated using AspenPlus RADFRAC model.

2.2 Ethylene Production from Ethane Steam Cracking

Ethane steam cracking occurs at high temperatures (approximately 800°C) in reactor tubes, where steam-diluted alkanes are converted, leading to homogeneous pyrolysis. Steam-cracking reactions are commonly described by using complex kinetic models, such as free-radical chain mechanism. Many parameters influence the performance of the process and the product distribution, including the partial pressures of the feedstock and steam, the residence time, and the process temperature (profile) in the reactor. In a typical steam cracking operation conversion with ethane as the feedstock can reach 70%, with olefin yields of ~50%. In naphtha crackers, the single-pass conversion yields are lower. Due to the high temperature of the reactions (1100 °C) and the highly reactive streams, the specification of suitable equipment materials becomes critical.

The entire process is grouped into three major sections, as shown in the Figure 3: pyrolysis (green color), compression (blue), and cooling and separation (orange). The model is mainly adapted from a published study (Thiruvenkataswamy 2015).

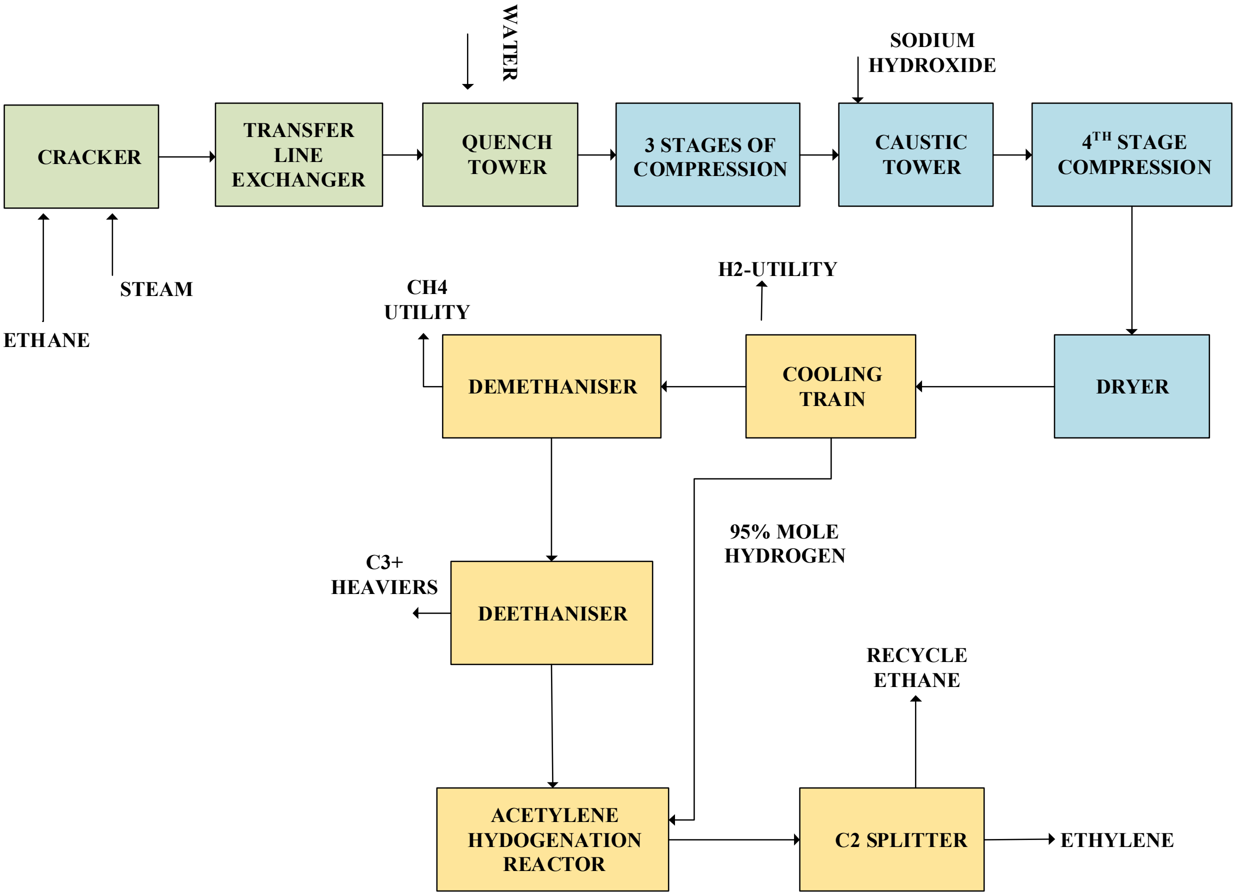

Figure 3. Block diagram of ethane steam cracking process.

The pyrolysis section, furnace, or cracker is where the ethylene product is formed by subjecting the ethane feed to high temperatures at low pressure. First, the feed ethane and steam are preheated to the initial cracking temperature (500–680°C). Subsequently, the mixed stream is fed into a high-temperature reactor (750–875°C) with residence times of 0.1–0.5 s to complete steam pyrolysis. External heat is usually provided by burning natural gas, where the radiant tubes (or coils) have different arrangements (split coil or parallel). Due to the high reactivity of the product, the effluent must normally be quenched in the quench tower within 0.02–0.1 s to avoid product degradation via side reactions.

A complex set of reactions based on free-radical mechanisms are usually applied to explain the process chemistry of thermal steam cracking of ethane in the pyrolysis furnace. Many studies report on investigating the thermal cracking of ethane to analyze the product-yield patterns and conversion of ethane through the furnace tubes. Under high temperatures and low pressures, ethane undergoes a dehydrogenation reaction to primarily form ethylene and hydrogen. Other primary products include methane, acetylene, propylene, propane, and butadiene. Sundaram and Froment (1977) reported that the products are obtained as result of complex combination of 42 free-radical steps. For the processes referenced (Thiruvenkataswamy 2015, Azmi and Aziz 2017, Sundaram and Froment 1977), only eight main reactions that allegedly define the net effect of the chemistry are considered out of all the reactions. They are given as follows:

i. $C_2H_6 \rightleftarrows C_2H_4 + H_2$

ii. $2C_2H_6 \rightarrow C_3H_8 + CH_4$
iii. $C_3H_8 \rightarrow C_3H_6 + H_2$
iv. $C_3H_8 \rightarrow C_2H_4 + CH_4$

v. $C_3H_6 \rightleftarrows C_2H_2 + CH_4$

vi. $C_2H_2 + C_2H_4 \rightarrow C_4H_6$
vii. $2C_2H_6 \rightarrow C_2H_4 + 2CH_4$
viii. $C_2H_6 + C_2H_4 \rightarrow C_3H_6 + CH_4$

The net effect of these reactions is endothermic; hence, external energy must be supplied to maintain the temperature of the reactor in order to increase yield of ethylene. This is accomplished by indirect-fired heaters, where heat release from combustion of fuel is used to heat the reaction mixture, which passes through the tubes fixed along the walls of the furnace. The main dehydrogenation reaction takes place in the temperature range of 750–850℃ at low pressures of about 1.5–3.5 bar (Thiruvenkataswamy 2015; Azmi and Aziz 2017; Sundaram and Froment 1977). The residence time of the reaction mixture in the cracker coils is about 0.1–0.5 s. Ethane is injected along with steam to reduce the partial pressure of hydrocarbons which, in turn, reduces the rate of decomposition of hydrocarbon products to coke at high temperatures. According to Sundaram and Froment (1977), steam-to-hydrocarbon ratio of range 0.3–0.45 is suggested for the process.

For this comparative analysis, a 60% single-pass conversion of ethane is assumed, which is in accordance with the literature (Thiruvenkataswamy 2015; Azmi and Aziz 2017; Sundaram and Froment 1977). Accordingly, the percentage conversions calculated from reaction kinetic data for the above eight reactions are shown in Table 2. These values are used for simulating the cracker reactor using RSTOIC. The calculated steam cracking yields obtained are shown in Table 3 (Froment et al. 1976).

Table 3. Conversions assumed for ethane cracking reactions.

Reaction	**Conversion %**	**Conversion of Limiting Reactant**
i. $C_2H_6 \rightleftarrows C_2H_4 + H_2$	56	Ethane

ii. $2C_2H_6 \rightarrow C_3H_8 + CH_4$	1.4	Ethane
iii. $C_3H_8 \rightarrow C_3H_6 + H_2$	35	Propane
iv. $C_3H_8 \rightarrow C_2H_4 + CH_4$	39.3	Propane
v. $C_3H_6 \rightleftarrows C_2H_2 + CH_4$	65	Propylene
vi. $C_2H_2 + C_2H_4 \rightarrow C_4H_6$	40	Acetylene
vii. $2C_2H_6 \rightarrow C_2H_4 + 2CH_4$	0.6	Ethane
viii. $C_2H_6 + C_2H_4 \rightarrow C_3H_6 + CH_4$	2	Ethane

Table 4. Product composition/yield (by wt.%) of ethane steam cracking

Components	**Modeled Pyrolyzer Yield**
Ethane	40
Ethylene	52.4
Hydrogen	3.8
Methane	2.6
Acetytlene	0.08
1-But-01	1.04
Propane	0.03
Propy-01	1.1

After exiting the pyrolysis section, cooled cracker products are compressed in stages to the desired pressure in order to effectively separate the ethylene from other components. First, the product stream is compressed by three stages of compression systems, each of which consists of a compressor, a cooling-water heat-exchanger intercooler to cool the compressed gases back to 40℃, and a flash drum to separate the gases from condensed liquid. Then, caustic scrubbing is used to remove acid gases and any residual moisture. Next, the gas is further compressed in the fourth-stage compressor to 36 bar and cooled to 15℃. The final step in this section is an adsorption-tower dryer where any residual moisture is removed in the gas stream before it enters the following cryogenic separation. Moisture and impurities are removed prior to the cryogenic section to avoid the formation of solid CO_2 or ice that can block equipment.

Next the gases enter the cooling and separation section. First, the tail gas enters a cooling-train system to effectively separate hydrogen from rest of the product gases. The cooling train consists of three stages of cooling, where each stage includes three heat exchangers and one flash drum. The three stages of cooling reduce the temperature to -29℃, -74℃ and finally -124℃, respectively. A hydrogen gas stream of 95 mol% is obtained after the third flash, and the rest hydrocarbons pass to the separation section.

The separation process consists of distillation and absorption. Front-end demethanizer and tail-end acetylene hydrogenation are used as the separation scheme in the reference steam-cracking process, where the methane and residual hydrogen are removed first, and followed by other, heavier products. The acetylene in the residual stream is reduced (hydrogenated) to ethylene, which is then separated during the separation section. The obtained ethylene achieves a purity of 99.9 wt%.

2.3 Modeling Results for Ethylene Production from Steam Cracking

The data for steam cracking, including energy consumption and operation information, are obtained from Thiruvenkataswamy (2015) and are summarized in Table 4. For the steam-cracking process, a steam-to-hydrocarbon ratio of 0.35 is used; a 60% single-pass conversion of ethane is assumed, resulting in a 40% single-pass ethylene yield.

As demonstrated in Figure 4, of the three main sections, the pyrolysis section is the biggest energy consumer, taking up 50% of overall energy consumption, followed by compression and then separation. The overall energy-requirement rate is about 3,554 million BTUs/hour, and the overall SEC is 37.5 MMBTU/metric tonne of ethylene produced.

Table 5. Energy requirement for each unit operation for the steam cracking process

Section	Unit	Type of Utility Used	MMBTU/tonne	MMBTU/hr
Pyrolysis	Feedstock Preheater	CH_4	7.376	699
	Cracker	CH_4	7.355	697
	Transfer line exchanger	cooling water	4.094	388
Compression	Recirculation Heater	cooling water	2.870	272
	Interstage cooler	cooling water	1.847	175
	Compressor	Power	5.255	498
Separation	Cool train	Refrigerant	1.055	100
	Reboiler	Steam	3.757	356
	Condersor	Refrigerant	2.818	267
	Acetylene Preheater	Steam	1.076	102

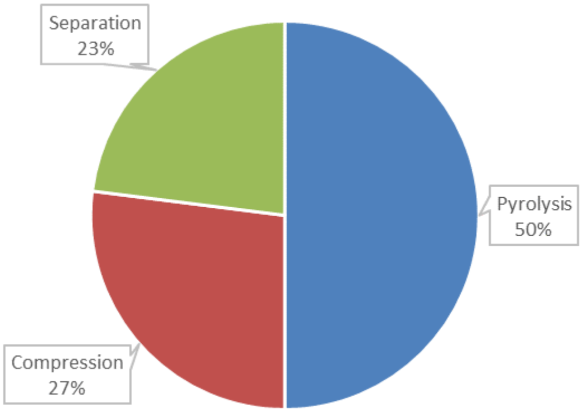

Figure 4. Specific-energy requirement of major sections for an ethane steam cracking process.

2.4 Modeling of the ENDP Process for Ethylene Production

The ENDP process flow diagram is shown in Figure 5 for nuclear-integrated ethylene production from ethane, which mainly consists of the following five process sections:

1. Electrochemical reactor
2. Compression and cooling
3. Distillation separation
4. Membrane separation
5. Refrigeration

Compared with the reference steam-cracking process, the electrochemical-reactor unit operation is unique to the ENDP process. The ENDP cell construction is similar to a solid-oxide electrolysis cell. Electricity is applied to assist in the dehydrogenation of ethane to form ethylene, which results in a lower operating temperature of 400–550℃, compared to 750–850℃ for the reference steam-cracking process. The separation schemes for the two processes are similar. However, both membrane separation and cryogenic distillation are applied in the ENDP process while only cryogenic-distillation systems are used for the reference steam-cracking process. Membrane separations were modeled in the ENDP process in an attempt to show further energy-reduction possibilities. Heat from a nuclear reactor is used to preheat all streams entering the ENDP reactor, and electricity from a nuclear reactor is applied to heat the ENDP reactor to power the compression and to be used in the refrigeration system. The major process operations are briefly described below. For each description, the name capitalized and enclosed in parentheses corresponds to the name of the unit block within the AspenPlus process model in Appendix A.

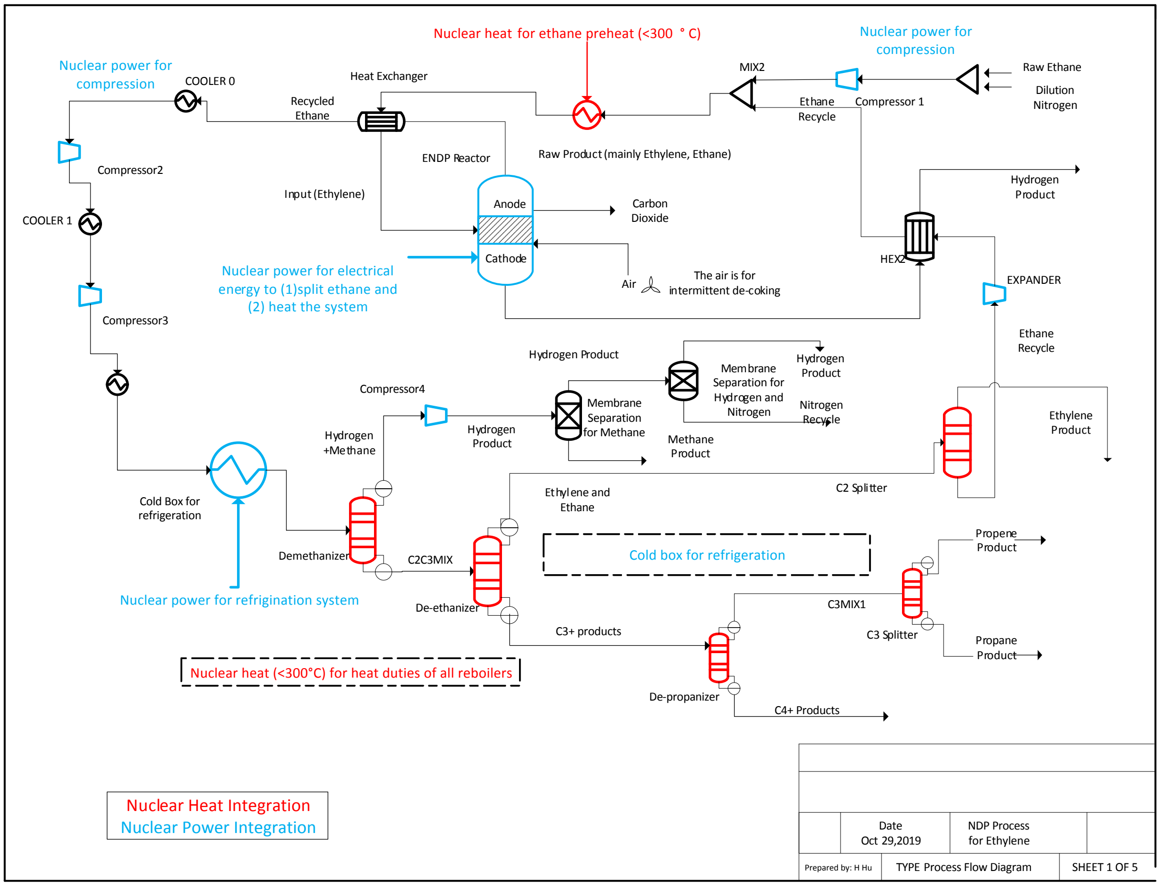

Figure 5. Simplified process-flow diagram for ethane to ethylene via ENDP process.

2.4.1 Ethane Feed and Dilution Nitrogen Compression and Preheat by Nuclear Steam (NUHEAT)

Steam is used to dilute ethane in conventional steam-cracking processes in order to reduce the partial pressure of hydrocarbons, the number of condensation reactions, and the rate of decomposition of hydrocarbon products to coke at high temperatures (Ranjan et al. 2012). Nitrogen is injected along with ethane in the ENDP process in lieu of steam for the same reasons. Based on the ENDP laboratory results, a ratio of 0.33 of nitrogen to ethane is applied in this analysis for both current and future cases. For comparison, the ratio of steam to ethane is 0.3–0.45 in steam-cracking processes (Rosli and Aziz 2017, Sundaram and Froment 1977). The feed-ethane and nitrogen come into the model at 20℃ and 20 psi and are subsequently compressed to 36 psi for downstream operation.

Low-pressure steam (at 275℃) from an NPP is used to preheat the feed gas. This low-pressure steam is also applied to other sections of the ENDP process to provide heating duties as required. The feed ethane combines with recycled ethane, the pressure of which is adjusted to be 36 psi before it is preheated to 265℃ by the steam from an NPP.

2.4.2 Reactions inside the ENDP Reactor (ELECTROR) for Ethylene Production

The feed ethane with dilution nitrogen is further preheated by the ENDP-reactor product stream and combined with recycled ethane before feeding into the ENDP reactor, which operates at 550°C and 30 psi. The electrochemical reactor, referred to as ELECRTOR in the simulation process, is modeled using an AspenPlus RSTOIC module. Its energy requirement includes thermal energy for maintaining operating temperature and reactions heat, and electrical energy for reaction. These thermal and electrical energy can be calculated theoretically as shown in Appendix C. In this study, all the required energy for the ENDP reactor are provided via electrical route, whose amount is determined from AspenPlus simulation.

The kinetic reactions in the ENDP reactor are proposed by the six reactions listed in Table 5. Reaction (i) is the main route for ethylene production, and proposed Reaction (vi) is the route for coke formation. In Reaction (i), ethylene forms on the anode side, and hydrogen forms on the cathode side after migration of hydrogen ions through the electrolyte. All other reactions occur as side reactions on the anode side. Thus, nearly pure hydrogen is formed on the cathode side, but hydrogen is also produced on the anode side as a result of side reactions.

Table 6. Reactions and corresponding conversions inside the ENDP reactor.

Reaction number	**Stoichiometry**	**Fractional conversion**		**Conversion of limiting reactant**
		ENDP current	**ENDP future**	
i	$C_2H_6 = C_2H_4$ (Anode) + H_2 (Cathode) (Ethylene Production)	0.363	0.56	Ethane
ii	$2C_2H_6 = C_3H_8 + CH_4$	0.02	0.02	Ethane
iii	$C_3H_8 = C_3H_6 + H_2$	0.8	0.8	Propane
iv	$2C_2H_4 = C_4H_8$	0.23	0.05	Ethylene
v	$C_2H_6 + C_2H_4 = C_3H_6 + CH_4$	0.032	0.07	Ethylene
vi	$CH_4 = C + 2H_2$ (Coke Formation)	0.07	0.05	Methane

The ENDP reactor is the core unit operation in this process. A depiction of the ENDP reactor is shown as Figure 5, where ethylene is produced on anode side, and hydrogen is produced on the cathode side. Hydrogen produced from reaction (i) is pure because it is the only theoretical product at the cathode. In order to represent the ENDP reactor in the modeling space, additional separate units had to be added that would not exist in an actual plant. For modeling purposes, the ENDP reactor is represented as three units instead of one in the AspenPlus simulation (as shown in Appendix A): (1) the ENDP reactor modeled using a RSTOIC reactor (ELECRTOR) where the six reactions in Table 5 take place; (2) a separator to separate anode products (ethylene, etc), the cathode product (H_2) and solid carbon "coke" (RECSEP) and; (3) a combustor for decoking via a combustion process introducing air to burn formed coke inside the ENDP reactor. These three separate units in the model represent a single ENDP reactor. Decoking would be accomplished by combustion of the coke particles that form as a result of Reaction (vi) in Table 5. During decoking, heated air is introduced into the ENDP reactor to burn the coke from the reactor surfaces (the COMBUST unit).

Laboratory Results: The single-pass ethylene yield in laboratory results varied with operating temperature and applied current. At 550°C, the single-pass ethylene yield at the anode side was reported as 25.7 wt% at the applied current of 40 mA/cm^2 as shown in Table 6, which also lists other product yields. These values are used for validating the simulated results of the ENDP reactor using RSTOIC module. It is worth noting that the yields listed in Table 6 are for the anode side. Most of the hydrogen produced in the ENDP reactor is on the cathode side, which is not included in the yields presented in Table 6. The fractional conversion for each reaction in the ENDP (shown in Table 5) is optimized in order to assure that the obtained simulated product yields agree with the experimental results. Table 6 demonstrates that the simulated results for ethylene, ethane, and C_{3+} heavy hydrocarbons match well with laboratory results with a variance of less than 0.01%.

With recycling and system integration, the overall ethylene yield for the ENDP current case is calculated from the AspenPlus simulation as 65%. By contrast, ethane steam cracking holds a 52.4 and 85% of ethylene yield for single pass and overall process, respectively (Thiruvenkataswamy 2015). The ENDP process is newly developed, so the single-pass ethane conversion inside the ENDP reactor is relatively low. This conversion is expected to increase as further development is done.

Table 7. Product composition (reactor yield) data of ENDP reactor at anode side at 550°C (hydrogen produced at the cathode is not included in these yield results).

Components	**Experimental result, wt%**	**Simulated result, wt%**	
	ENDP current	**ENDP current**	**ENDP future**
Ethane	61.8	61.8	40
Ethylene	25.7	25.9	48.5
Hydrogen	2.2	1.2	0.12
Methane	0.7	0.7	2.2
1-But-01	9.6 (sum for all C3+)	10.4	9.18
Propane			
Propy-01			

The ENDP process is endothermic and thus requires external thermal energy to maintain the temperature of the reactor and external electrical energy to increase the yield of ethylene. Detailed calculations on the amount of energy required is presented in Appendix C, "ENDP Reactor Design." Nuclear electricity is utilized in this study to provide energy for both resistive heating to maintain the ENDP reactor temperature at 550°C as well as the electricity for the electrochemical process for splitting ethane to produce ethylene.

2.4.3 Cooling and Compression (HEX, COOLER, COMPRESSOR)

The ENDP product stream of nearly pure hydrogen from the cathode side does not receive any further treatment. The anode product consisting mainly of ethane (70wt%), ethylene (12.5wt%), nitrogen, C_{3+} hydrocarbons, methane, and hydrogen leaves the ENDP reactor at a temperature of 512°C. The stream is cooled in a heat exchanger (i.e., HEX1) by preheating the feed and recycled ethane. Then the product stream is further cooled to 1°C before entering the two-stage compression system with interstage cooling using cooling water and refrigeration. The first compression stage increases the pressure to 80 from 25 psi, then the stream is cooled to 1°C and sent to the second-stage compression, where the pressure increases to 150 psi and the stream is subsequently cooled to 1°C again. The reference steam-cracking process had a similar design by using three-stage system (Thiruvenkataswamy 2015).

2.4.4 Refrigeration System (COLDBOX)

The ENDP product stream leaving Compressor 2 is cooled, by cooling water and refrigeration, to 1°C. Then the COLDBOX refrigeration system is responsible for further cooling the stream to a temperature that allows cryogenic distillation to be feasible. In this system, a three-step cascade process is modeled using phase separators, throttle valves (i.e., Joule-Thomson valves), and coil-wound heat exchangers, as shown in Figure 6. The refrigeration system is required to further reduce the temperature for downstream cryogenic separation in liquid condition at the specified temperature (i.e., -150°C) and pressure (145psia).

The following are specifications for the COLDBOX design:

- Use of mixed refrigerant (MR) to better match cooling curves
- Use of a multistage/cascade process to reach cryogenic temperatures
- Use of a coil-wound heat exchanger for heat transfer.

As shown in Figure 6, recycled refrigerant, at a temperature of 1°C, is compressed to 30 atm through four-stage compressions, each stage consisting of one compressor and one cooler to reduce the compressed-gas temperature back to 1℃. The refrigerant is then sent to the first-phase separator, where gaseous refrigerant is separated from liquid refrigerant. The liquid refrigerant is throttled to a temperature of -44°C, at which point it mixes with a cold stream from HEX1. This stream then enters HEX0 to provide cooling duty for the ENDP product stream. The gaseous refrigerant from PS1 enters HEX0 and HEX1 where it is cooled even further, until it reaches PS2. The liquids stream from PS-203 is throttled to a temperature of -59°C and mixed with the refrigerant stream leaving HEX3. This stream, at a temperature of -78°C, provides cooling duty to HEX1 and HEX2. On the other hand, the gaseous refrigerant from PS2 is further cooled in HEX2, and then expanded to a temperature of -83°C to provide cooling duty to HEX3, which provides cooling duties for all the condensers of distillation columns.

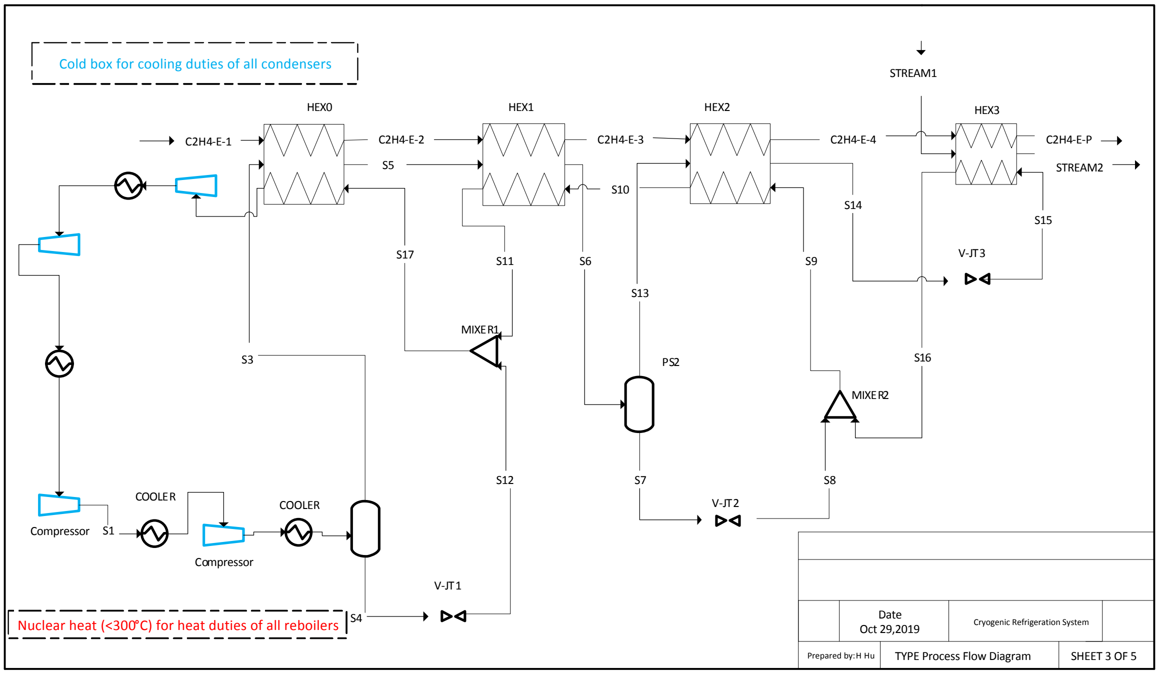

Figure 6. PFD for the cryogenic refrigeration system.

2.4.5 Product Separation by Distillation Columns

The separation section consists of traditional cryogenic-distillation separation and membrane separation. Considering the recent development of membrane separation for some gas separations and the high energy requirements of cryogenic distillation, membrane separation systems are employed to separate hydrogen, methane, and nitrogen in order to reduce overall energy consumption. Other hydrocarbon separations are conducted via cryogenic-distillation columns, which include five columns (Figure 5).

The product stream leaving the COLDBOX process enters the first distillation column (demethanizer) at -150℃ and 145 psi. Methane, nitrogen, and hydrogen are separated from the other hydrocarbons as the distillate product, which will be treated by membrane system as described in the following section. The bottom product from the demethanizer consists of ethane, ethylene, and other C_{3+} hydrocarbons (including propane, propylene, and butane).

Distillation towers are sized using AspenPlus after the desired separation scheme has been successfully modeled. All columns are sized using bubble-cap trays with a spacing of 2 ft to allow for potential frothing as a safety factor. Appendix F, "Distillation Column Separation Design," provides more details on design methods and more-complete sizing information.

2.4.6 Product Separation by Membrane System

The light products from the demethanizer mainly include methane, nitrogen (dilution stream), and hydrogen, with trace amount of ethylene (<0.1%).

The dilution nitrogen needs to be separated and recycled back to the ENDP reactor. Despite the design complexity and compression requirements, multistep, multistage membrane systems are the lowest-cost nitrogen-removal technology in many applications (Lokhandwala et al. 2010). To date, 12 membrane-based systems for nitrogen removal during natural-gas processing have been installed (Lokhandwala et al. 2010; Baker and Low 2014). It was reported that methane-selective membranes are generally preferable and membranes with high permeances and methane/nitrogen selectivity of approximately 3–3.5 were developed (Lokhandwala et al. 2010). This selectivity is modest, so commercial systems often require multistage- or multistep-process designs. Hydrogen separation using a membrane system is also deployed in commercial applications. The details of this section on membrane separation can be found in Appendix G, "Membrane Separation Design."

In addition, if ethylene is used as the starting chemical for many other products, particularly the widely utilized polyethylene, polymer-grade ethylene (≥99.95% pure) must be obtained. The well-established industrial cryogenic-distillation process requires large distillation columns and high reflux ratios because of the similar sizes and volatilities of C_2H_4 and C_2H_6 (Li et al., 2018). It is highly desired to achieve cost- and energy-efficient C_2H_4/C_2H_6 separation, which has been recently highlighted as one of the most important industrial separation tasks for future energy-efficient separation processes (Li et al. 2018). Membrane process, among other alternatives including adsorbent-based gas separation, through pressure swing adsorption (PSA), and temperature swing adsorption, is a promising technology to replace the traditional cryogenic distillation and thus to fulfill the energy-efficient separation economy.

Therefore, the feasibility of employing a membrane separation for ethane and ethylene is also analyzed for both ENDP current and future cases. And the detailed membrane design can be found in Appendix G.

In summary, the above processes in an ENDP system are shown in the process-flow diagram obtained from AspenPlus simulation as shown in Figure 7. From the simulation, process data, and mass and energy balance, design specifications are obtained for each equipment. All unit operations are simulated and optimized to account for balanced energy consumption, product purity, and operation and design considerations. For columns, compressors, and heat exchangers, primary design data are fetched from AspenPlus models. The assumptions made for design of certain class of equipment are listed below.

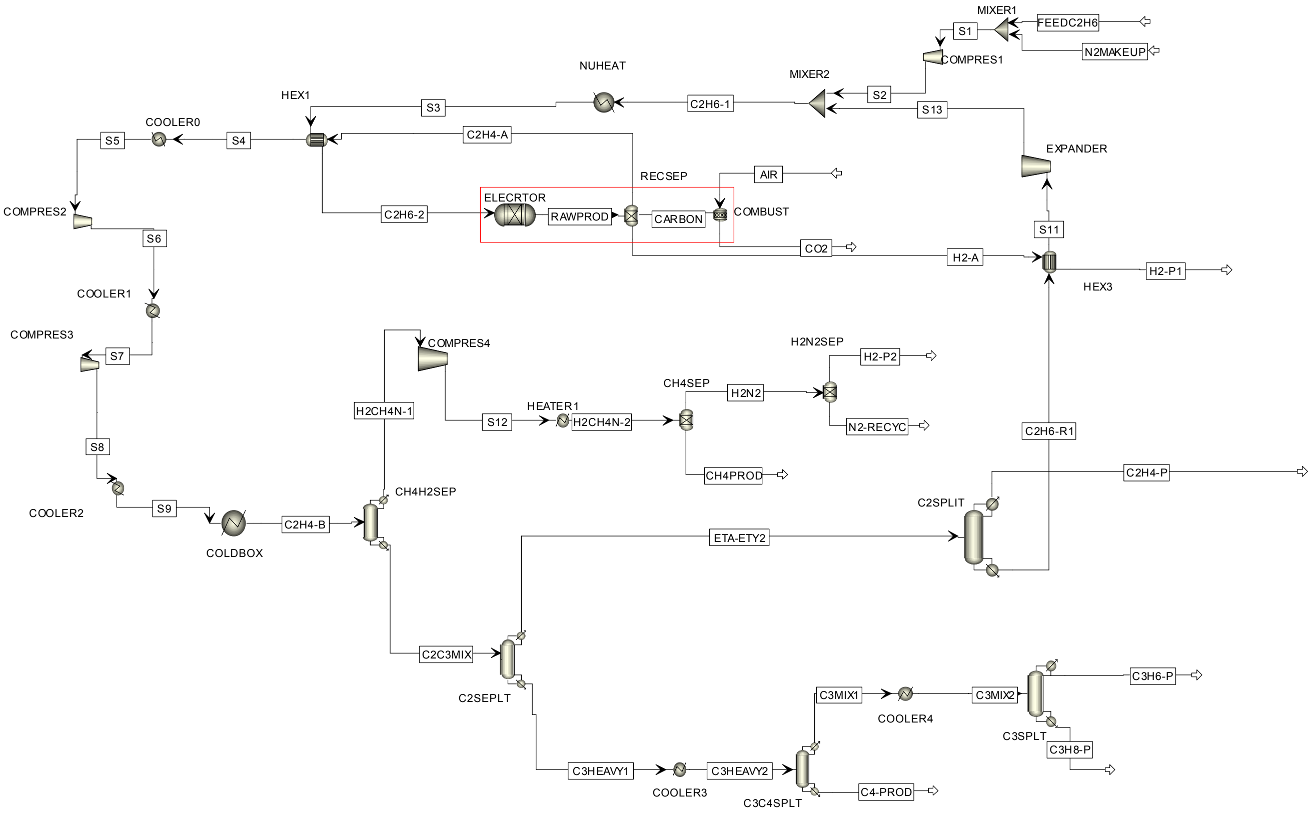

Figure 7. Process-flow diagram of ENDP process from AspenPlus simulation.

2.4.7 Assumptions and Conditions for AspenPlus Simulation

Assumptions for the simulation were:

1. Ethane feed is available at 20°C and 20 psi.
2. The nuclear low-pressure steam is available at 275°C.
3. The actual ENDP reactor is modeled by three separate units: a reactor using RSTOIC model; a separator for separating hydrogen at the cathode side and other products at anode side; and a reactor for decoking by burning the produced carbon.
4. There is no further reaction among the products leaving the ENDP reactor; products leave the reactor at temperature below 600°C.
5. Pressure drop of heat exchangers is 5 psig for the hot side and 3 psig for the cold side.
6. All heat exchangers are assumed to be shell-and-tube type. Heat-transfer areas and other specifications are calculated from AspenPlus. A minimum temperature approach of 10°C is assumed for refrigeration operations and other exchangers.
7. The rule of thumb for maximum heat-transfer area is 1000 m^2. Any heat exchanger exceeding this value was split accordingly into parallel heat exchangers.
8. The maximum allowable column diameter is assumed to be 6 m. Any column exceeding this value is split accordingly into parallel columns.
9. Sizing of reactors and columns is obtained from AspenPlus and is manually compared to literature

values. The residence time for half-full flash vessels is assumed to be 5 min according rule of thumb (Coker 2007). Approximate volume of column is calculated using the formula:

Volume = π * (Column diameter)^2 * Height of column / 4
Height of column = No of trays * tray spacing + 10 feet
Default tray spacing of 0.6096 m (2 feet) is assumed for columns.

10. All products recovered from distillation are based on minimum 99% mass recovery except for propane and propylene separation, which are 90%.
11. Compression ratio of compressors was assumed in such a way so as not to exceed compressor-outlet temperatures greater than 150°C to avoid formation of polymers that plug equipment.

Heating duties are provided by steam from an NPP. Cooling duties are provided by cooling water except for the cooling and separation section. MRs are used for cooling purposes in cooling and separation section.

2.5 Modeling Results for Ethylene Production from ENDP Process

Considering that the ENDP process is still in the early TRL research stage, two economic cases were evaluated: Case 1, a *predicted current* case based on 2019 lab-scale technology, and Case 2, a *projected future* case based on expected technology advancements. The future case is hypothetical, showing performance increases that could potentially be realized if progress is made in technological and process areas mentioned in the basis below. The main performance difference for the two cases is the conversion for each reaction inside the ENDP reactor increases for the *projected future* case, as shown in Table 5. The ethane conversion in the reaction (i) in Table 5 is increased to 56%, compared to 36.3% in the current case (Table 5). This results in a much higher single-pass ethylene yield as shown in Table 6, 48.5% compared to 25.7% for current case (Table 6). Consequently, the overall ethylene yield for the future case increases to 75.8%, compared to 65% of the current case. The chosen ethane conversion of 56% for the ENDP future case is according to data of a steam-cracking reference process (Thiruvenkataswamy 2015).

The basis for the projected improvement for Case 2 is current laboratory results and understanding of both ENDP and traditional steam-cracking processes. As discussed, ENDP is an emerging technology, newer than steam cracking, where materials and the overall process have been extensively optimized with a decades-long track record of reliable operation. Analogously, the ENDP process will improve as it is scaled and optimized. At the current stage, widespread technology adoption and gradual market penetration for ENDP will require aggressive and continuous innovation of materials and processes to improve the yield of ethylene and enhance the lifetime of system components. Specifically, there are three areas where technical challenges exist and are, if improvement is achieved, most likely to produce increased performance. These are targeted for research and improvement: electrocatalysts, cell component materials, and overall process optimization.

1. *Development of Electrocatalysts*. Electrocatalysts at elevated temperatures are thermally activated; consequently, some problems associated with elevated temperatures occur that result in thermodynamic limitations. It is thus necessary to develop novel electrocatalysts that can maximize the benefits of electrochemistry by efficiently enabling the flow of electrons, while also enabling the desired reactions. This would result in “true” electrocatalysis and high conversion of ethane at reduced temperatures where side reactions, catalyst deactivation, and coking will be remarkably suppressed.
2. *Cell Component Materials*. One technical opportunity is to improve the proton-transference number of the electrolyte and the resulting Faradaic efficiency in a reducing atmosphere. This will allow the electrochemical cell to operate at much-higher current densities with sufficient proton flux. The benefits include not only a faster driving force to move the reaction forward, but larger quantities of hydrogen produced at the cathode side as well as distinctly reduced separation cost when co-occurrent

hydrogen at the anode side is too hard to separate.

3. *Overall Process Optimization*. In addition to the development of the materials and catalysts, it is crucial to investigate the effects of all operating conditions on the ultimate yield of ethylene and lifetime durability. Specific design of the electrochemical cell and stack, scaling, and modularity, as well as engineering of feedstock and downstream distribution are each important for achieving an economically viable operation. It is expected that an effective combination of experiments, modeling, and technoeconomic analyses is the key for further development and implementation of ENDP to meet the projected targets, which are attainable.

Both cases were modeled in AspenPlus according to the conversions and yield percentages obtained from lab data for Case 1 and projected for Case 2. The feed rate of ethane in the model was scaled to match the reference industrial-scale steam cracking process.

The ENDP-process model, as described in the previous sections, provides the overall mass and energy balance. The SEC for each major section of the ENDP process is shown in Table 7 for both the current and future cases.

Table 8. Energy requirement for each unit operation of the ENDP process simulated by AspenPlus

			Project Current Case		**Project Future Case**	
Section	**Unit operation**	**Type of utility used**	**MMBTU/ tonne**	**Q, MMBTU/hr**	**MMBTU/ tonne**	**Q, MMBTU/hr**
Pyrolysis	Feedstock Preheater	NPP Low Steam	2.300	167	1.032	87
	ENDP electricity	Electricity	6.280	456	5.659	477
	Compressor 1	Electricity	0.136	10	0.117	10
	Expander	Electricity	-0.137	-10	-0.076	-6
Compression	Interstage coolers	Cooling Water	1.212	88	0.546	46
	Compressor	Electricity	0.977	71	0.509	43
Separation	COLDBOX compressors	Electricity	9.594	697	5.062	427
	Condersors (1,2,5)	Electricity	6.300	458	5.576	470
	Condersors (3rd and 4th)	Cooling Water	0.275	20	0.403	34
	Reboilers	NPP Low Steam	4.476	325	4.615	389
	Coolers	Cooling Water	0.069	5	0.059	5
	Compress4	Electricity	0.129	9	0.059	5
	Membrane Preheater2	Steam	0.110	8	0.036	3

Figure 8 shows that, of the three main sections for the current case, the separations section is the biggest energy consumer, accounting for 66% of overall consumption, followed by the reaction section (27%), and then compression. The overall energy-requirement rate is about 2303 MMBTU/hour, and the overall SEC is 31.72 MMBTU/metric tonne of ethylene produced. The performance of the ENDP process improves significantly in the future case, but demonstrates a very similar trend. The separation section still consumes the most energy, taking up 67% (Figure 8), followed by reaction (29%) and compression. The overall SEC decreases by 25% to 23.6 MMBUT/tonne ethylene produced. This is mainly due to the increased ethylene yield in the future case, which reduces the recycle volume of gases, then increases the overall energy efficiency of the whole process. This is different from the conventional steam-cracking process.

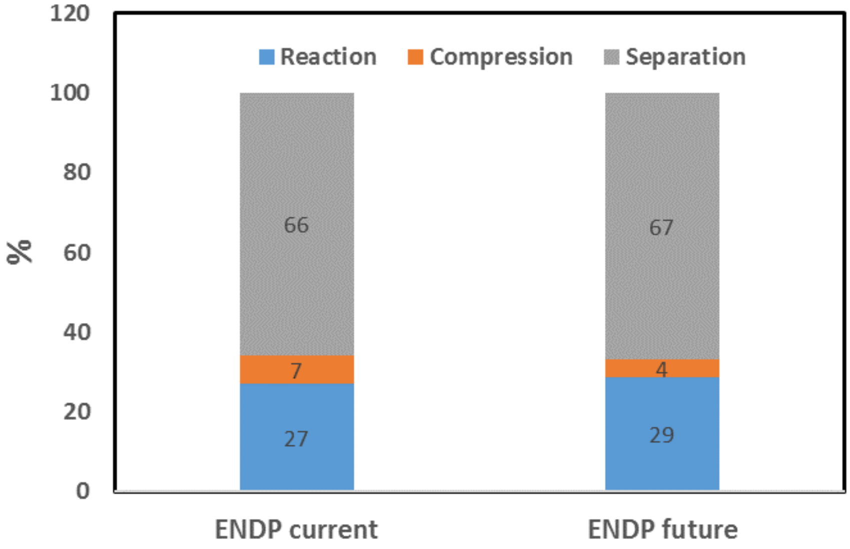

Figure 8. Specific-energy requirement of major sections for the ENDP process.

Table 8 provides a brief summary for the two processes: ENDP and steam cracking. The overall energy requirement of steam cracking is about 1.6–1.8 times higher than that of ENDP. This is mainly due to the high operating temperature of steam cracking process.

Table 9. Process result summary for steam-ethane cracking and electrochemical NPD ethylene production

Parameter	Unit	Steam Cracking	ENDP Current	ENDP Future
Annual Ethane Feed Rate	Metric Tonne/Yr	978,492	972,360	972,360
Annual Production Rate Of Ethylene	Metric Tonne/Yr	830,132	636,125	738,407
Ethylene-Product Purity	%	99.90	99.90	99.90
Annual Production Rate of H_2	Metric Tonne/Yr	0[a]	62,835	64,824
H_2 Product Purity	%	-	99.90	99.90
Ethane Single-Pass Conversion	%	**60**	**38**	**60**
Ethylene Single-Pass Yield	%	**52.4**	**25.7**	**48.5**
Process Yield of Ethylene	%	85	65	76
Operating temperature	°C	850	550	550

Overall Specific-Energy Consumption	MMBTU/Metric Ton Ethylene	37	32	24
Overall Energy-Requirement Rate	MMBTU/hr	3,554	2,303	1,989
Operation Hours Per Year	Hour	8760	8760	8760
Plant Lifetime	Year	20	20	20

[a] The off-gas generated from steam cracking process, including hydrogen, methane, acetylene, propylene, propane, and butadiene, are considered in the form of equivalent of natural gas for heating and are balanced in the final energy of fuel required.

[b] The thermal energy for ENDP to maintain reactor temperature can be provided via thermal energy by burning natural gas, or can be applied by electrical heating system. Thermal energy is applied in here.

Figure 9 and Figure 10 demonstrate the major energy contribution for both steam-ethane cracking and ENDP processes for ethylene production. The pyrolysis reaction contributes the biggest part of energy requirement for steam cracking, taking 50% of total energy requirement, while the reaction in ENDP is less than 30%. The total energy consumption of compression and separation for both ENDP and steam cracking are very close, within 5%. This indicates that the reaction performance of ENDP is superior to steam cracking.

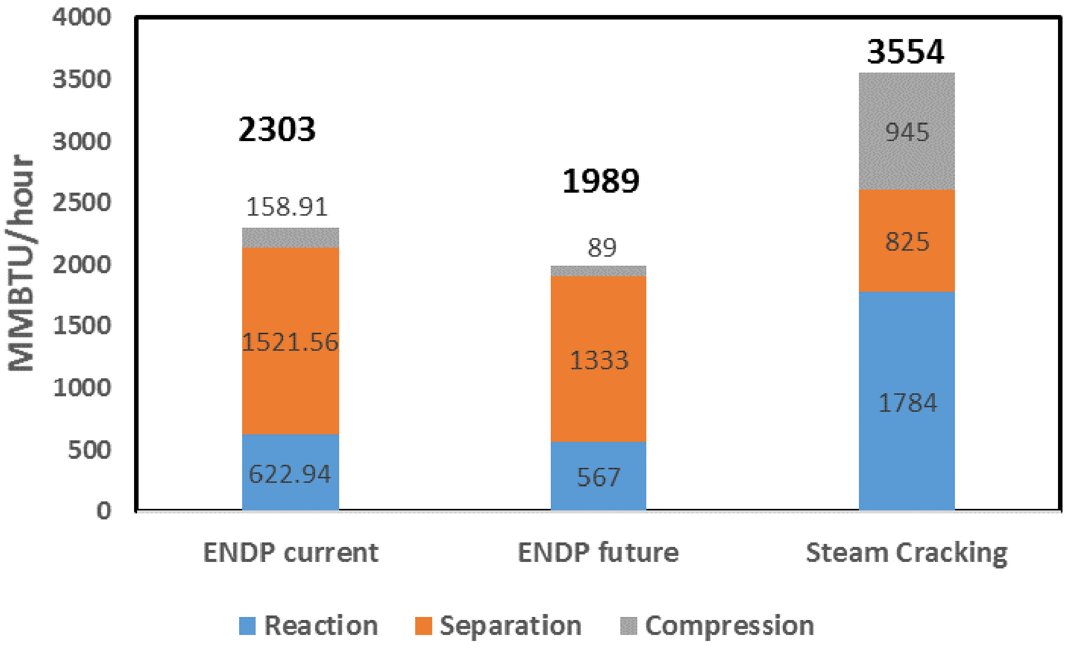

Figure 9. Energy use for steam-ethane cracking versus the ENDP process.

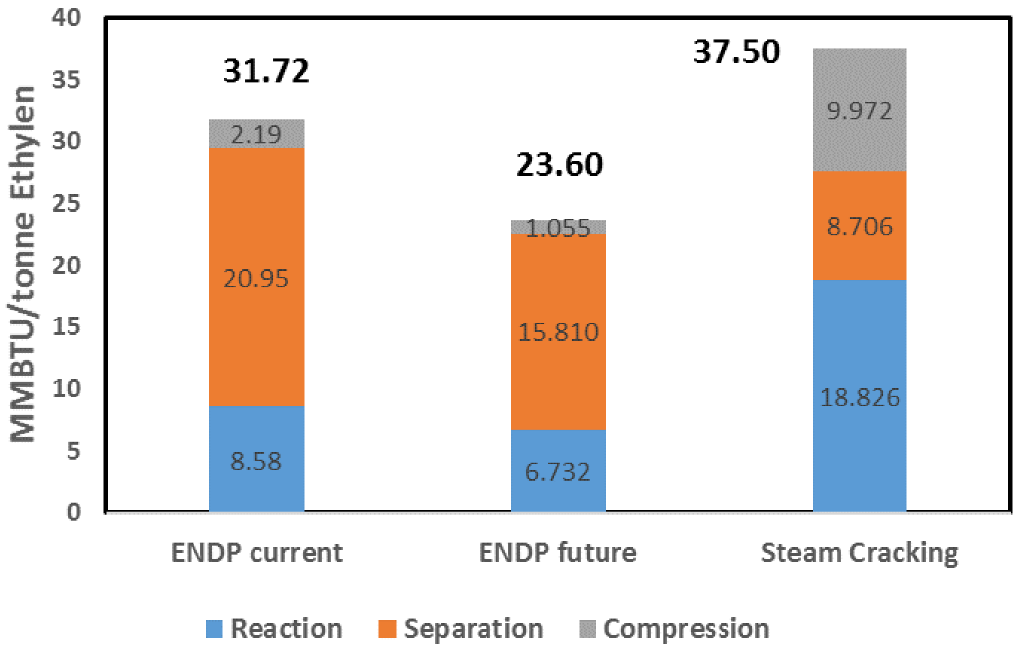

Figure 10. Specific-energy use for steam-ethane cracking versus the ENDP process.

Table 9 lists the mass balance for some important streams of the ENDP process. Because an annual operation time of 8760 hours was used in the reference steam-cracking process (Thiruvenkataswamy 2015), it was also used for the electrochemical ENDP process for consistency.

Table 10. Mass balance for selected main streams for the ENDP current case simulated by AspenPlus.

	Units	**S2**	**C2H6-R1**	**C2H6-2**	**RAWPROD**	**C2H4-A**	**H2-A**
ETHANE	kg/hr	111000.00	177289.86	288289.86	177368.69	177368.69	0.00
OXYGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE	kg/hr	0.00	779.20	779.20	73352.89	73352.89	0.00
HYDROGEN	kg/hr	0.00	0.00	0.00	7155.86	3577.93	3577.93
NITROGEN	kg/hr	37000.00	0.00	37000.00	37000.00	37000.00	0.00
METHANE	kg/hr	0.00	0.00	0.00	2200.80	2200.80	0.00
1-BUT-01	kg/hr	0.00	0.00	0.00	22634.92	22634.92	0.00
PROPANE	kg/hr	0.00	0.40	0.40	538.69	538.69	0.00
PROPY-01	kg/hr	0.00	45.09	45.09	5738.68	5738.68	0.00
CARBON	kg/hr	0.00	0.00	0.00	124.02	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flows	kg/hr	148000.00	178114.56	326114.56	326114.56	322412.61	3577.93
Temperature	C	63.78	-35.75	537.41	550.00	550.00	550.00
Pressure	psia	36.00	130.00	33.00	30.00	30.00	30.00

Table 10. continued

	Units	C2H4-B	H2-P2	C2C3MIX	C3HEAVY 1	ETA-ETY2	C2H4-P
ETHANE	kg/hr	177368.69	0.00	177368.63	34.06	177334.57	44.71
OXYGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE	kg/hr	73352.89	0.00	73351.22	0.27	73350.96	72571.75
HYDROGEN	kg/hr	3577.93	3229.08	0.00	0.00	0.00	0.00
NITROGEN	kg/hr	37000.00	366.30	0.00	0.00	0.00	0.00
METHANE	kg/hr	2200.80	0.00	0.99	0.00	0.99	0.99
1-BUT-01	kg/hr	22634.92	0.00	22634.92	22634.92	0.00	0.00
PROPANE	kg/hr	538.69	0.00	538.69	538.29	0.40	0.00
PROPY-01	kg/hr	5738.68	0.00	5738.68	5693.59	45.09	0.00
CARBON	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flows	kg/hr	322412.61	3595.38	279633.13	28901.13	250732.00	72617.45
Temperature	C	-150.00	20.00	-37.80	52.31	-40.91	-59.79
Pressure	psia	145.00	80.00	144.00	144.00	130.00	110.00

3. ECONOMIC ASSESSMENT

3.1 Capital Cost Projection

Again, given that the ENDP process is still in the early research stage, with no pilot- or commercial-scale system available, the *projected current* Case 1 and *predicted future* Case 2 are extrapolated from technology demonstrated only at the laboratory scale. For cost estimating, the ENDP process can be compared to the existing high-temperature electrolysis (HTE) process utilizing solid-oxide electrolytic cells (SOEC) because of the electrochemical similarities in cell-stack construction, reactions, and operation. Furthermore, the specific hydrogen production rate per reactor area is comparable for these two processes, 0.037 g/cm2-hr in ENDP vs 0.035 g/cm2-hr for HTE. Then considering the similarity of ENDP and HTE, it is reasonable to estimate the ENDP capital costs using the Department of Energy (DOE) hydrogen analysis (H2A) model with high-temperature electrolysis configurations (NREL H2A 2018; Peterson and Miller 2017). The H2A model is a model developed by the National Renewable Energy Laboratory (NREL) to analyze hydrogen production by any method in a standard and comparable way. The proposed ENDP-plant economic analysis was performed with the economic-parameter specifications as summarized in Table 10, which are consistent with other analyses. For all cases considered, the minimum selling price (MSP) that achieves a 12% IRR for the given CAPEX and OPEX is calculated. This IRR value is typically reported in the open literature as it serves as a common reference for investor decisions.

Table 11. Summary of financial model input parameters the ENDP future ethylene plant economic model.

Description	Value	Comments
Ethylene selling price	\$0.44/kg [\$0.2/lb]	Fixed selling price at plant gate
Nominal IRR	12%	
Electricity price (\$/MWh-e)	30	
Debt to equity ratio	60% debt, 40% equity$^{\alpha}$	
Debt interest rate	5%$^{\alpha}$	Debt backed under Federal Loan Guarantee Program
Debt period	10 years	Debt backed under Federal Loan Guarantee Program
Overall tax rate	424.8%	20% federal; 6% state
Capital depreciation schedule	Standard Modified accelerated cost recovery system (MACRS) depreciation method	Depreciation method, with a property class of 5 years
Labor cost	\$50,000/employee	This is the average value for all staff
Land	\$1.848M	
Working capital	8.3% of total capital investment	
Salvage value	None	
Plant construction period	3 years	Percent capital invested is 8, 60, and 32 for the 1st, 2nd, and 3rd years, respectively
Startup time	1 year	Operating costs and revenues during startup are 75% and 50% of the total

		values, respectively
Plant life and analysis period	20 years	Excluding construction time

According to published data, the total capital investment (TCI) for a 1.5 mtpa steam-ethane cracker on the U.S. Gulf Coast was about at $2.13 billion in 2016 (Petrochemical Update 2016), and $1.43 billion for a 1 mtpa cracker (Petrochemical Update 2016, 2017, 2018). A detailed item breakdown for the main sections of a steam cracking plant is listed in Table 11.

Table 12. Detailed capital costs items for steam cracking [PetroChemical Update 2018].

Major Equipment	**Bulk Materials**	**Indirect**
Columns c/w trays	Removals/Demolition	Detail Design/Engineering
Drums/vessels	Site Earthmoving	Contingency
Pumps	Piling	EP Fee
Compressors/Fans/Blowers	Buildings	Fringe Benefits/Payroll Burdens
Heat Exchangers	Concrete	Consumables/Small Tools
Tanks	Refractory/Fireproofing	Field Supervision and Expenses
Material Handling	Structural Steel/Platforms	Support Labor
Water Treatment	Piping system	Construction Equipment Rental/Fuel
Miscellaneous Equipment	Insulation	Contractor Fee
Electrical Equipment	Electrical/Instrumentation	Project Management and Controls
Instrumentation Devices (Tagged)	Painting/Coatings	Field Establishment(Trailer, Toilets)
Freight	Other Misc. Costs	Other Misc. Costs

As demonstrated in Figure 11, the major equipment (containing 70 columns, 67 vessels, and several hundred other pieces of equipment as in Table 11) represents about 29% of TCI while bulk materials and indirect costs account for 28% and 43% of TCI, respectively (Petrochemical Update 2018). These same percentages were applied for the calculation of capital costs of the ENDP plant.

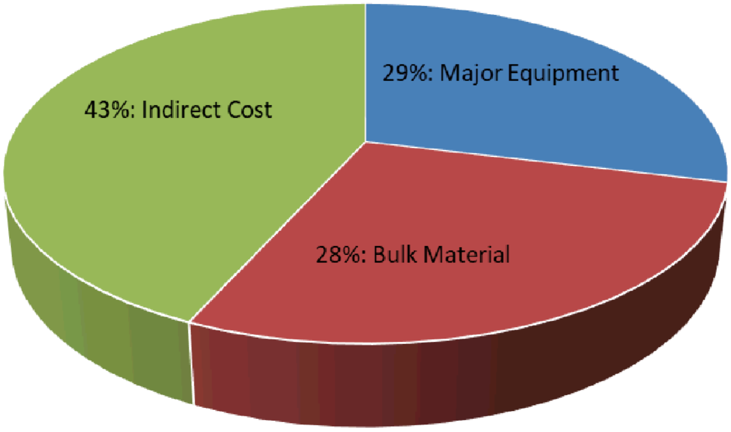

Figure 11. Capital cost distribution for a steam cracking.

The major equipment of the ENDP process can be grouped into five sections: ENDP-reactor system, compression and cooling, membrane separation, distillation separation, and the refrigeration system. The ENDP reactor system is the core process, and its cost is obtained using the H2A model for HTE SOEC (NREL H2A 2018, Peterson and Miller 2016). Because stack capital costs of $287/kW and $99/kW for SOEC electrolyzers were specified in the H2A model for SOEC's current Case 1 and future Case 2, respectively, these values are used to obtain capital costs of the ENDP reactor (NREL H2A 2018, Peterson and Miller 2016, James and DeSantis 2015). The costs for compression/cooling and distillation sections are obtained from AspenPlus Economic Analyzer, v10. For the refrigeration system, the cost information from existing work (Lindgren 2013) is used as the baseline. Other studies report higher refrigeration costs (Humbird et al. 2011), so a contingency factor of 1.5 is applied to assure conservatism (Peters and Timmerhaus 2013). The costs for membrane separation were based on various industrial references, the detailed design information for which is found in Appendix G.

The costs for major equipment for both ENDP cases were then calculated. The detailed costs for each unit operation of the ENDP process are listed in Appendix I, "Cost Information." The overall cost for major equipment in the ENDP current case is $165 million dollars, while it decreases 40% to $100 million dollars for the future case, based on expected technology development (Table 12).

Table 13. Major equipment list of ENDP process.

	Millions of Dollars		**%**	
	ENDP Current	**ENDP Future**	**ENDP Current**	**ENDP Future**
Refrigeration	13	10	8	10
Distillation	8	6	5	6
Membrane	6	6	4	6
Compression	35	23	21	23
ENDP reactor	102	55	62	55
Total	164	100		

Figure 12 shows the cost contribution from each major section. Both the current and future case demonstrate similar trends. The ENDP reactor system contributes the biggest cost share, up to 62% and 55% of TCI for the current and future case, followed by compression at 20%, and 23% for the current and future cases, respectively.

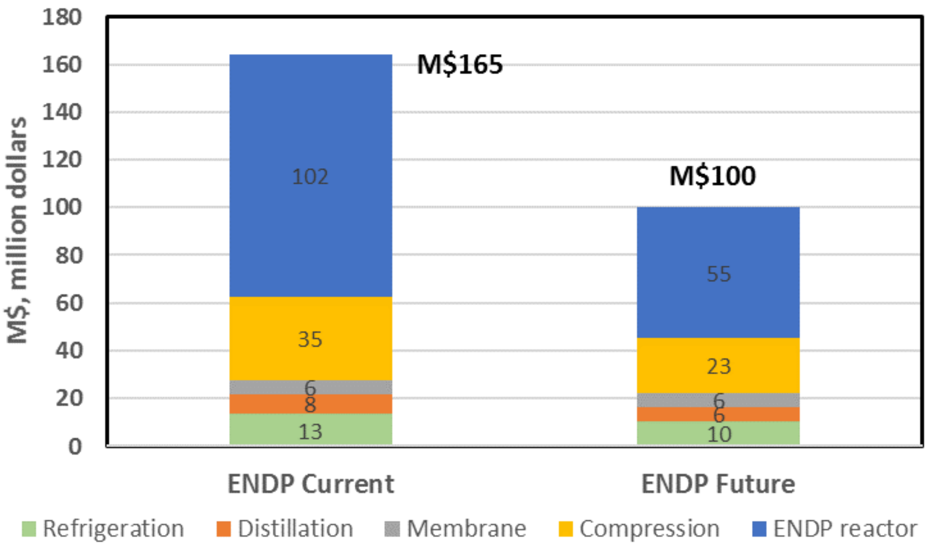

Figure 12. Cost contribution of major section of an ENDP plant.

Table 14. TCI for both steam cracking and ENDP processes (costs are in millions of dollars).

	ENDP current	**ENDP future**	**Steam Cracker**
Major Equipment	165	100	325
Bulk Materials	155	95	300
Indirect Cost	250	150	485
TCI	**570**	**345**	**1,110**
Ethylene, tonne/yr	636,125	738,407	830,132
$/tonne Ethylene	896	467	1,337

The TCI costs are obtained and compared with those of conventional steam cracking (Table 13). The results plotted in Figure 13 provide a visual comparison of the relative costs. The TCI of the ENDP current case ($0.57 billion) is about half of that of the steam cracker ($1.1 billion), and it is projected to be less than one-third than that of the steam-cracking system for the future case by 2025.

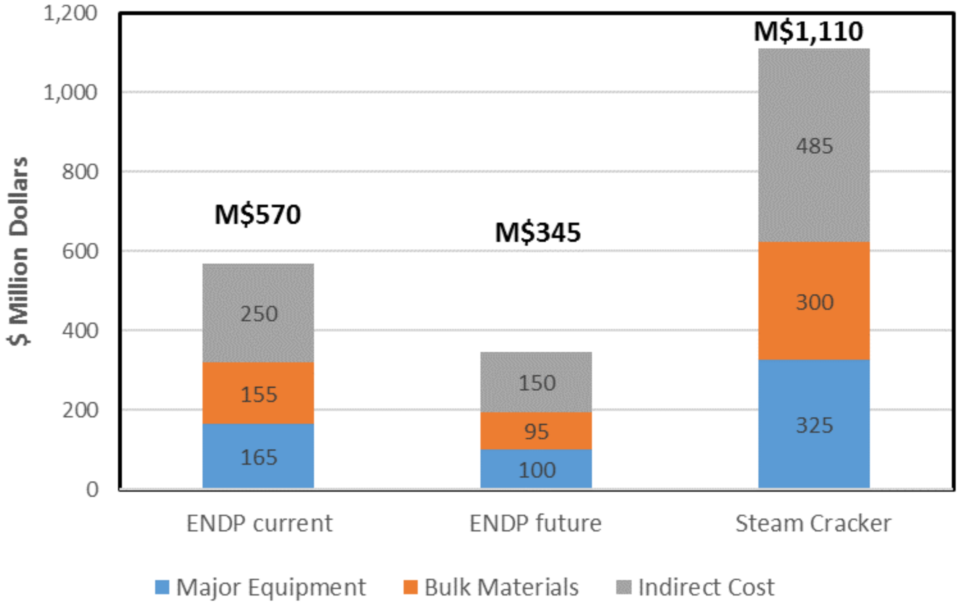

Figure 13. Capital costs for ENDP and steam-ethane cracking.

For comparison, the Lang-factor method was also used to estimate TCI based on major equipment (Turton 2010). An updated Lang factor of 3.28 (Wain 2014) was used to double check the TCI for ENDP. The result obtained with the Lang-factor method is less than 5% lower than that obtained from the method used in steam cracking (PetroChemical Update 2018). (See Table 14.)

Table 15. TCI calculation form Lang factor.

	ENDP current Million Dollars, M$	**ENDP future**
Major Equipment	165	100
TCI by PetroChemical	570	345
Lang Factor	3.282	
TCI by Lang Factor	542	328
difference, %	4.99	4.87

Considering the assumptions listed in Table 10, the financing debt is 60% at a loan rate of 5% for 10 years. The total interest is calculated and the TCI including interest are summarized in Table 15.

Table 16. Project financing and TCI with interests for ENDP process.

	ENDP current	**ENDP future**
Plant financing debt/equity of TCI	60%	40%
Loan amount	$342,000,000.00	$207,000,000.00
Loan rate	5.00%	5.00%

Term (years)	10	10
Interest per month	0.417%	0.417%
Number of payment periods	120	120
Total Interest Paid	($93,292,875)	($56,466,740)
Total paid	$435,292,875	$263,466,740
Payment (monthly)	$3,627,441	$2,195,556
TCI, including interest	$663,292,875	$401,466,740
Total capital charges ($/yr)	$22,109,762.48	$13,382,224.66
Total capital charges ($/dt)	$1,042.71	$543.69
Capital charge rate (%)	5.08%	5.08%

3.2 Operating Costs Projections

Detailed energy projections categorized by utility are shown in Table 16 for conventional steam-ethane cracking (Thiruvenkataswamy 2015).

Table 17. Detailed energy consumption for steam-ethane cracking by type of utility.

	Unit operation	**type of utility used**	**MMBTU/tonne**
Thermal	Feedstock Preheater	Natural gas	7.376
	Cracker	Natural gas	7.355
	Reboiler	steam	3.757
	Acetylene Preheater	steam	1.076
	Subtotal		**19.564**
	Transfer line exchanger	cooling water	4.094
Cooling	Recirculation Heater	cooling water	2.870
	Interstage cooler	cooling water	1.847
	Subtotal		**8.811**
Refrigeration	Cool train	Refrigerant	1.055
	Condenser	Refrigerant	2.818
	Subtotal		**3.873**
Compressor	Compressors	Electricity	5.255
	Non-electricity subtotal	32.249	
Total			**37.504**

Table 17 shows the energy utilization for ENDP process. For each tonne of ethylene produced, a steam cracker requires thermal and electrical energy totaling 37.5 MMBTU, which is slightly higher than 31.72 MMBTU of the ENDP current case. However, the energy requirement for ENDP future case drops 37% to 23.6 MMBTU as demonstrated in Figure 14. The energy requirement for the two processes are summarized in Table 17.

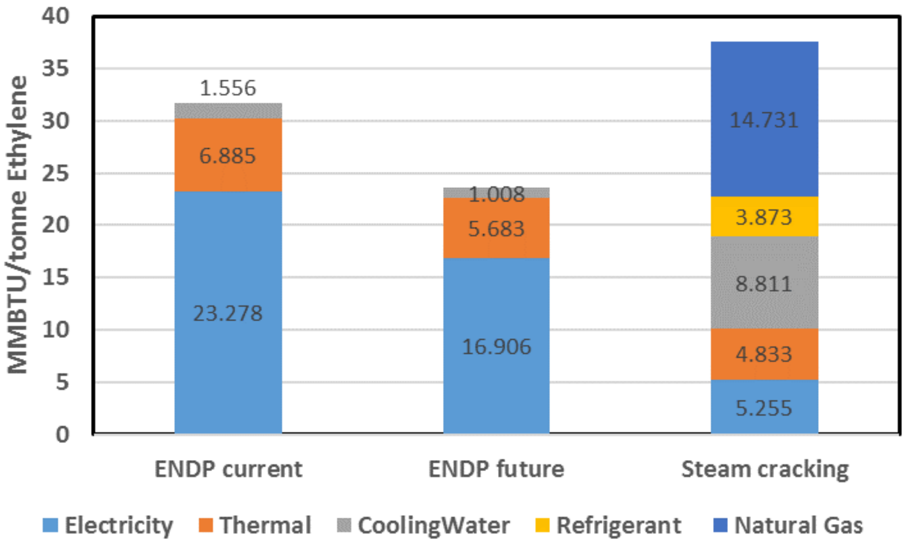

Figure 14. Energy section contribution for ENDP and steam cracking.

Table 18. Detailed energy consumption for ENDP process by type of utility.

			ENDP current	**ENDP future**
Section	**Unit operation**	**Type of utility**	**MMBTU/tonne**	
Pyrolysis	Feedstock Preheater	NPP low steam	2.300	1.032
	ENDP electricity	electricity	6.280	5.659
	Compressor1	electricity	0.136	0.117
	Expander	electricity	-0.137	-0.076
Compression	Interstage coolers	cooling water	1.212	0.546
	Compressor	electricity	0.977	0.509
Separation	COLDBOX compressors	electricity	9.594	5.062
	Condersors (1,2,5)	electricity	6.300	5.576
	Condersors (3rd and 4th)	cooling water	0.275	0.403
	Reboilers	NPP low steam	4.476	4.615
	Coolers	cooling water	0.069	0.059
	Compress4	electricity	0.129	0.059
	Membrane Preheater2	steam	0.110	0.036
		Total	31.720	23.596

It is worth noting that hydrogen generated on the cathode side in the ENDP process is pure; no further separation is needed. The off-gas generated from the steam-cracking process includes hydrogen, methane, and acetylene. This off-gas is generally burned to support process heating.

An overall-system energy balance can be obtained when the energy for feed input and product output are included. Table 18 summarizes the energy balances for the two processes and Figure 15 provides a visual representation. The ENDP future case demonstrates the highest overall-system energy efficiency at 80%, compared to 50% of steam cracking.

Table 19. Summary of energy input and output for steam-ethane cracking and ENDP processes.

		ENDP current	**ENDP future**	**Steam cracking**
		MMBTU/tonne C2H4		
Input	Electricity	23.278	16.906	5.255
	Non-electricity energy	8.442	6.691	32.249
	Ethane feed	68.392	58.919	52.739
Sum of input energy content		**100.112**	**82.515**	**90.243**
Output: product	Ethylene	45.250	45.250	45.250
	Hydrogen	11.243	9.992	
	Methane	1.788	2.393	
	Propane	0.561	0.253	
	Propylene	3.221	5.288	
	Butane (C4+)	13.305	2.448	
Sum of product energy content		**75.367**	**65.624**	**45.250**
System energy efficiency, %		**75**	**80**	**50**

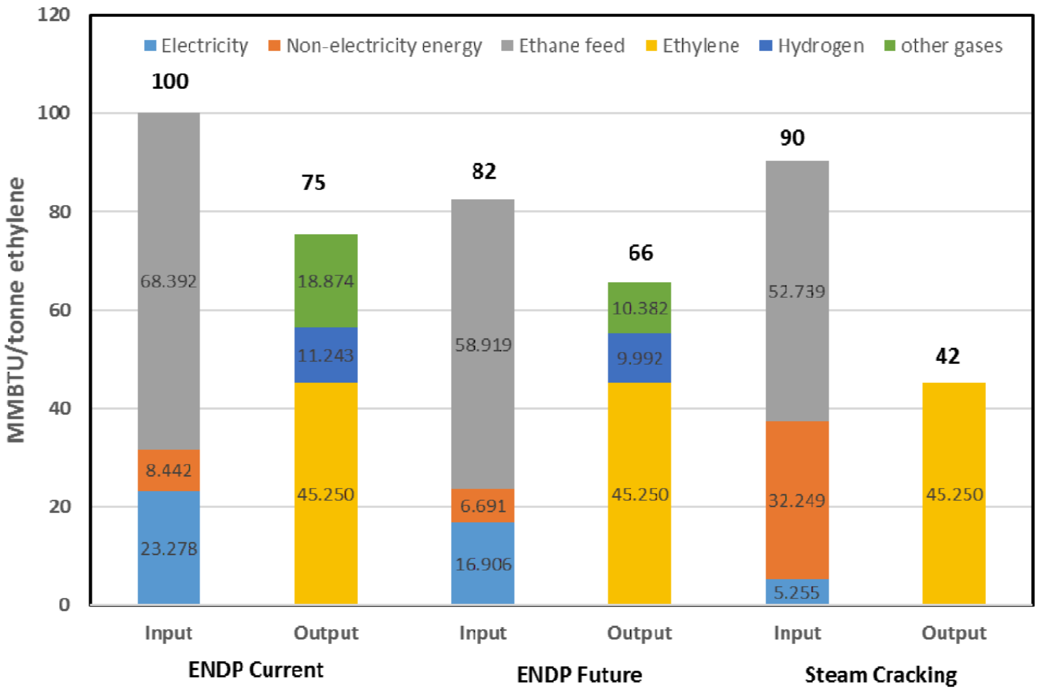

Figure 15. Energy input and output for ENDP and steam cracking.

Many elements influence the cost of manufacturing chemicals. According to literatures and industrial practices, the important factors are listed in Table 19 and are generally divided into three categories (Turton et al. 2010), among which the direct cost takes 90% of the total cost of manufacturing, and fixed cost and general expenses are for 3% and 7%, respectively (Turton 2010).

Based on the energy consumption described above, operating costs consist of feedstock (ethane), thermal energy, electricity energy, and labor cost for both of the processes analyzed. A breakdown of the estimated direct operating costs for the steam-ethane cracking process were projected from published data (Thiruvenkataswamy 2015) and are tabulated in Appendix I.

Table 19 lists relative costs of raw materials for both processes, which translate to the overall operating costs per tonne of product, listed in Table 20. The ENDP current case has the highest OPEX cost per tonne of ethylene at $665 million dollars compared to $579 million dollars for steam cracking, while the ENDP future case requires $535 per tonne ethylene. This is mainly due to the relatively low ethylene yield of the ENDP current case, and high electricity usage in both ENDP cases, taking 30% and 27% in ENDP current and future case, respectively. The ENDP current case requires an annual $423 million dollars for operating, whereas the cost is $480 million dollars for steam cracking. For ENDP future case, the cost is reduced to $395 million dollars per year.

Table 20. Factors affecting operating costs.

1	**Direct Operating Cost**			90%
	1)	Raw material		
	2)	Utilites		
	3)	Labor		
	4)	Waste treatment		
	5)	Maintenance and repair		
	6)	Operating supplies		
2	**Fixed Operating Cost**			3%
	1)	Depreciation		
	2)	Tax and insurance		
	3)	Plant overhead		
3	**General Operating Expenses**			7%
	1)	Administration cost		
	2)	Distribution and selling cost		
	3)	Research and Development		

Table 21. Summary of raw material costs for steam cracking and electrochemical NPD.

	Unit	**Value**
Electricity	$/kWh	0.03
Steam	$/tonne	20
	$/MMBTU	10.12
Natural gas	$/MMBTU	4
Cooling water		

	$/MMBTU	
Refrigeration	$/MMBTU	20
Ethane	$/kg	0.2

Table 22. Relative total operation costs (OPEX) summary for steam-ethane cracking and ENPD

Utility	**ENDP current**	**$/tonne ENDP future**	**Steam cracking**
Ethane feed	306	263	236
Electricity	205	149	46
Steam	70	58	49
Natural gas			59
Refrigerant			77
Cooling water	3	2	18
Labor	16	10	36
Total Direct	599	482	521
Fixed cost	20	16	17
General Expenses	47	37	41
Total OPEX	665	535	579

Figure 16 graphically compares the total operating cost per metric tonne of ethylene produced. ENDP current case is about 15% higher than the cost of steam-ethane cracking; however, the ENDP future case is 7% lower than that of steam cracking. Feedstock cost accounts for the biggest amount of the total operating cost for the processes, 51% and 45% for ENDP current and steam cracking, whereas it accounts for 55% for ENDP future case, indicating the higher overall-system energy efficiency.

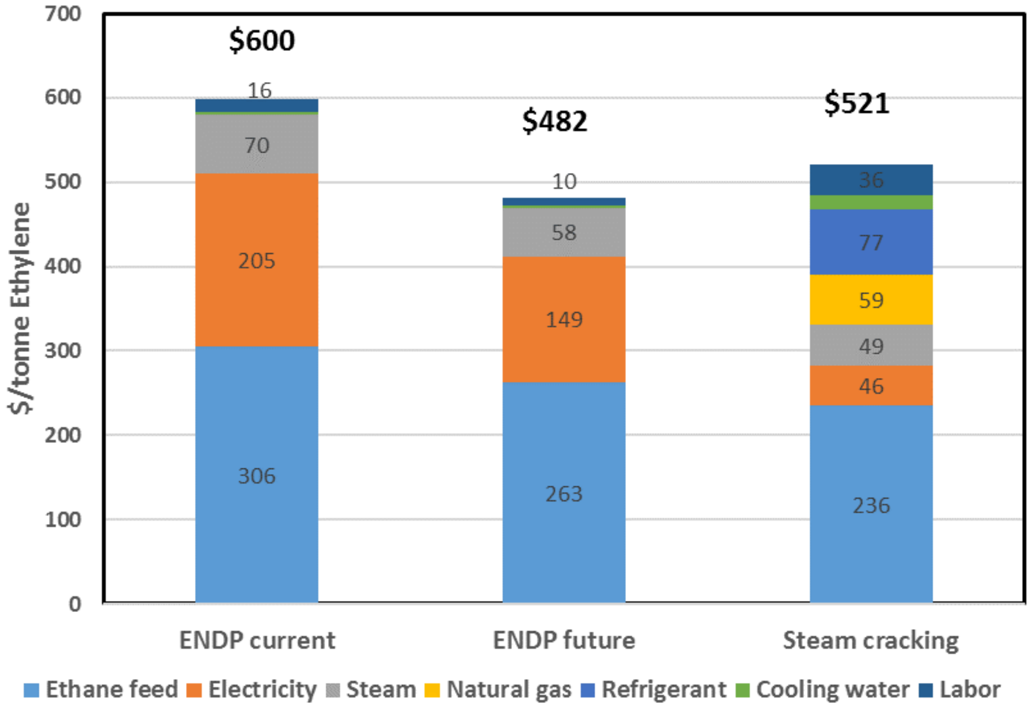

Figure 16. Relative direct operating costs for ENDP and steam-ethane cracking.

3.3 Estimation of Revenue

Annual revenues are estimated for all cases based on recent price data for the various products generated as summarized in Table 22. For the steam-cracking process in this report, the total off-gas generated constitutes of 12,259 Kg/hr of 54.79 mo % of hydrogen, 6.8 mol% of ethylene, 37 mol% of methane, and 1 mol% of ethane, which produces a combined heat duty of around 1189 MMBtu/hr and gives the credit of off-gas to energy cost. Therefore, they do not include revenue of byproducts. Then the only saleable product in the steam-cracking process is ethylene, which accounts for an annual revenue of $365 MM.

For the ENDP process, annual sales for the current case are estimated to be $500 MM each year, which is comparable to that of the future case, $521 MM per year. Both have over 42% higher revenue than does steam cracking. Of the saleable products for both the ENDP cases, ethylene yields the most profit, and hydrogen is the second highest seller annually. For the ENDP future case, ethylene ($325 MM) contributes 62% more than hydrogen ($258 MM), and the side products, methane, C_3, and C_{4+} account for the remainder.

Table 23. Revenue of saleable products.

	price	**ENDP current**	**ENDP future**	**Steam cracking**	**ENDP current**	**ENDP future**	**Steam cracking**
	$/kg	**Tonne/year**			**M$/year**		
Ethylene	0.44	636,125	738,407	830132	280	325	365[a]
Hydrogen	1.49	62,835	64,824		94	97	

Methane	0.20	24,072	37,396		4.81	7.48	
Propane	0.26	8,156	4,266		2.14	1.12	
Propylene	0.81	47,348	90,228		39	73	
C4+	0.41	197,678	42,223		82	18	
Total					**500**	**520**	**365**

[a]: The off-gas and byproducts generated in steam cracking is used as a credit to offset energy cost and is not shown here as product.

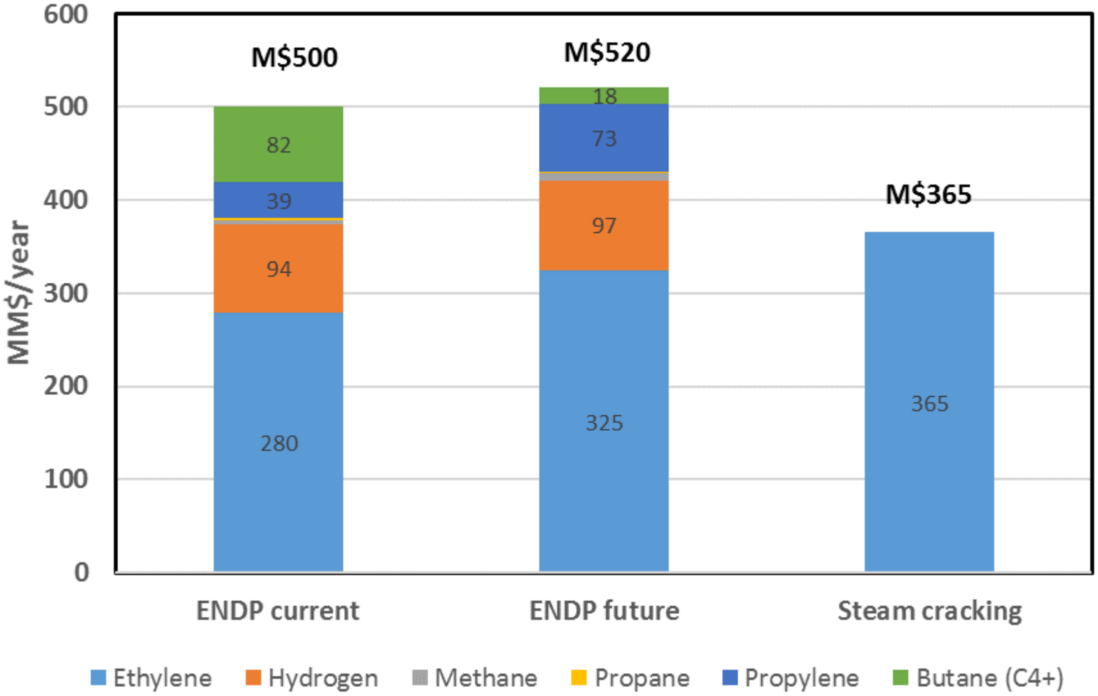

Figure 17. Revenue contribution from saleable products.

3.4 Economic Profitability Analysis

A variety of factors could dramatically impact the economic outcome of an ENDP process. As discussed in earlier sections on ENDP current and future cases, the single-pass ethylene yield of the ENDP reactor would be the biggest factor because a high single-pass yield reduces the overall system size by decreasing the total amount of recycle gases, which reduces the CAPEX and OPEX. In this and the following section, the economic profitability and sensitivity analysis of parameters of the ENDP future case are evaluated.

Three bases are commonly used for evaluation of a project profitability (Turton 2010):

1. Net present value (NPV) gives the present value of all payments and provides a basis of comparison for projects with different payment schedules but similar lifetimes. In making comparisons between projects, the larger the NPV, the more favorable the investment. It is one of the most widely used economic measures because it captures the time value of money, the value of investment incentives and variations in construction schedule, while allowing for price-forecast models that include cyclic behavior. The NPV can be represented as:

Where *is cash* flow in year *n*, t = project lifetime, and *i* is the discount rate as a decimal. There are

several drawbacks to NPV; it does not measure bang for the buck, and it cannot be optimized unless an upper bound is set to the plant size.

2. Discounted cash-flow rate of return (DCFROR)/IRR: interest or discounted rate for which the NPV of the project is equal to zero. This means that DCFROR represents the highest after-tax interest rate at which the project can break even. Often, corporation management will set an "internal" interest rate, which is the lowest rate of return that a company will accept for any new investment. If the DCFROR is greater than this internal rate, the investment is favorable. NPV and DCFROR are almost always used together. DCFROR is useful for comparing projects of different sizes and for comparing projects to other investments.
3. Discounted payback period (DPBP): the number of years required, after startup, to recover the fixed capital investment, (2) FCI, with all cash flows discounted back to time zero. The project with the shortest DPBP is the most desirable.

With an IRR of 12% and a selling price of ethylene at \$0.44/kg (\$0.2/lb), the anticipated NPV for this project is \$285 MM. This IRR value (12%) is typically reported in the open literature as it serves as a common reference for investor decisions. The DPBP is 5 years.

3.4.1 Net Present Value

The NPV for this project is expected to be \$285 MM. This accounts for many factors, including taxes (24.8% of the revenue), depreciation, an IRR of 12%, an ENDP reactor stack life of ten years and a selling price of ethylene at \$0.44/kg. Considering the 7 years of SOEC stack life in DOE studies (Peterson and Miller 2016) and the lower applied current density (40 mA/cm^2 vs 1 A/cm^2) and operating temperature (550℃ vs 850℃), ten years of ENDP reactor stack life is used for the discounted cash-flow analysis of the ENDP future case. The calculations involving depreciation use the 5-year MACRS schedule (Turton 2010). And the replacement capital cost is set as 10% replacement each year. Full calculations for the NPV are provided in Appendix I.

Figure 18 shows the discounted cumulative cash-flow diagram for the ENDP future case. The drop at Year -2 shows the land costs, the drop in Year 0 shows the working-capital and startup costs, and the drops between Years -2 and 0 are the fixed capital investment. The project begins at Year 0, but does not make a profit in its first year. Over the first year, the plant only produces half of its total capacity, but incurs all production costs, resulting in monetary losses. However, after the first year of production, the plant runs at full capacity. After six years, the depreciation allowance runs out, resulting in higher taxes and a reduced cash flow. The project breaks even in eight years. At the end of the project lifetime, the working capital and land are returned, resulting in an NPV of \$285 MM.

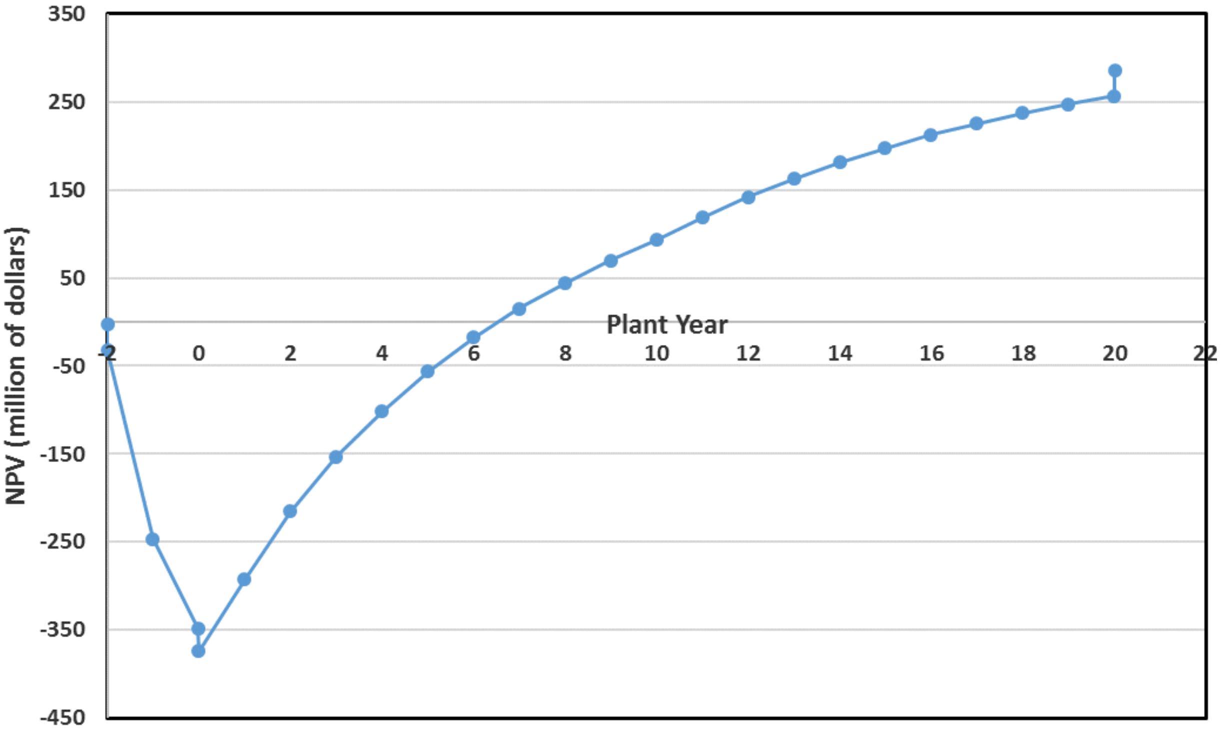

Figure 18. Cumulative cash-flow diagram for the ENDP future case for ethylene production.

3.4.2 Discounted Cash-Flow Rate of Return/ Internal Rate of Return

At each IRR, the product selling price that achieves an NPV of zero is called the MSP. At an IRR of 12%, the MSP of ethylene is $0.37/kg, which causes the project to achieve an NPV of $0 at the end of the plant lifetime. This makes it the highest interest rate and the lowest selling price that will allow the project to break even.

On the other hand, a low, average, and high ethylene selling price would result in different IRRs. Table 23 presents the summary of the IRRs with different ethylene selling prices. It is worth noting that the current industrial ethylene price is at $0.44/kg ($0.2/lbs), a historically record low price. At an ethylene selling price of $0.44/kg and an IRR of 12% the project achieves a positive NPV of $285 million. Figure 19 visualizes the effect of the ethylene selling price on IRR. Higher selling prices results in higher IRR.

Table 24. IRR results for different MSP for ENDP future case.

IRR	12%	22.5%	40.42%	72.5%
MSP of ethylene, $/kg	0.37	0.44	0.6	1

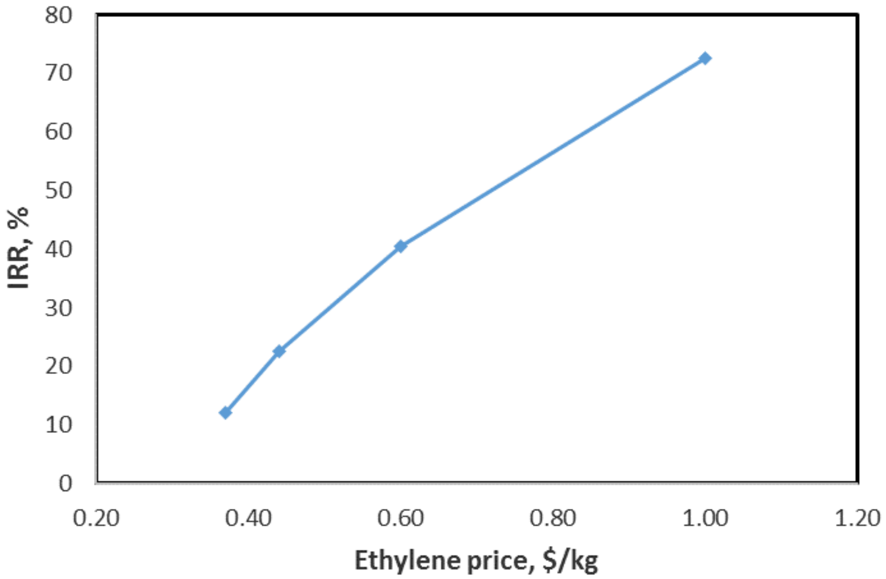

Figure 19. IRR vs ethylene MSP economic results with NPV set equal to zero for the ENDP future case.

3.4.3 Discounted Payback Period

The DPBP is eight years of operation. This means that the project recovers all capital and operating costs and begins making money after five years.

3.4.4 Discounted Cash Flow of Steam Cracking Process

For the steam cracking process, the MSP of ethylene is obtained at $0.88/kg for an IRR of 12% if only ethylene is counted as revenue, whereas it is $0.37/kg for the ENDP future case. The high MSP for steam cracking mainly because the byproducts including hydrogen, propylene, butane are not includes for revenue income. Table 3 shows that the yields for hydrogen, methane, propylene and butadiene are all higher than 1%, which are corresponding to a $119M as byproducts revenues (Table 27). When these revenues are included, the MSP of steam cracking is about $0.71, which is still almost double of that of ENDP future case. This is mainly due to the high capital cost of steam cracking ($1,110M), which is more than three times than that of ENDP future case.

Table 25. Byproducts revenue of steam cracking.

Products Revue	$/kg	tonne/yr	$/yr
Hydrogen	1.49	60,200	89,698,614
Methane	0.20	41,190	8,237,951
Propylene	0.81	17,426	14,115,412
Butane (C4+)	0.41	16,476	6,833,324
Total			119,000,000

3.5 Sensitivity Analysis

As demonstrated in Figure 16, feedstock cost accounts for the biggest amount of the total operating cost, 51% for ENDP current, following by electricity (34%). Hydrogen and propylene contribute 88% of coproduct revenue. In addition, the ENDP reactor is a big uncertainty for the process, since its costs are estimated based on H2A model for SOEC electrolyzers. Therefore, low, average (base), and high prices of these factors are applied for the sensitivity analysis of the ENDP future case as summarized in Table 25. The corresponding MSP of ethylene is calculated with an IRR of 12%. When one factor changes from low to high value, all other factors keep their base value. The gases prices are from EIA (2019a,b).

At the base value of each factor, the MSP is calculated as $0.37/kg ethylene produced. Figure 20 demonstrates the percentage change versus the baseline price by varying each factor from low to high range. The price of feed ethane is the biggest influencer, causing 35% variation on the MSP of produced ethylene from every $0.1/kg change of ethane, followed by the prices of electricity, hydrogen and propylene.

Table 26. Summary of various prices of key factors for sensitivity analysis for ENDP future case.

	Ethane	**Electricity**	**H_2**	**Steam**	**ENDP Stack**	**Propylene**
Price	$/kg	$/MMh	$/kg	$/MMBTU	$/kW	$/kg
Low	0.1	15	1	5	100	0.35
Base	0.2	30	1.49	10.12	150	0.81
High	0.3	45	2	15	200	1

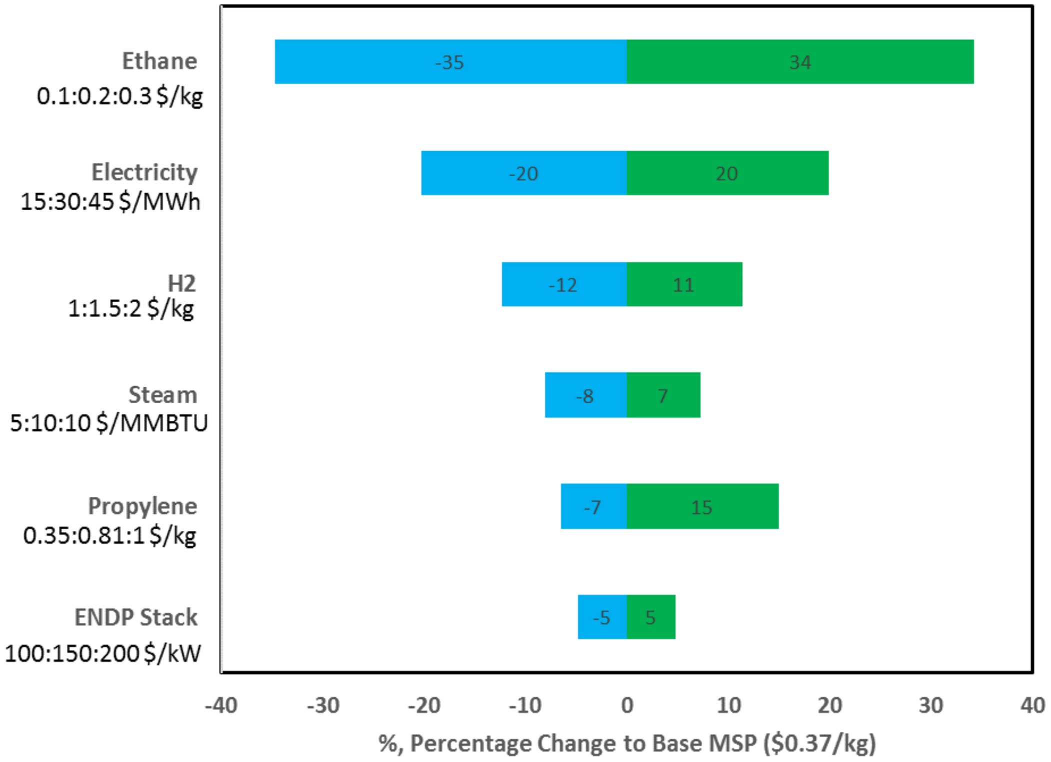

Figure 20. Tornado diagram for the minimum, base and high values of factors affecting MSP of ethylene for ENDP future case. IRR set to 12%.

3.6 CO_2 Emissions

For the ENDP process, very little CO_2 emissions are produced. CO_2 emissions come from two sources: burning fuel to provide reaction heat and the electricity requirement of the reactor. If nuclear power is used to provide reaction heat through resistive heating and for all electricity requirements of the reactor, then carbon emissions are reduced to near zero. The ENDP process has a remarkable advantage relative to reducing CO_2 emissions. Figure 21 plots the output from the AspenPlus model for ENDP with data obtained from literature for steam-ethane cracking (Ding 2018; Ren 2006). The steam-cracking process emits 1.47 tonnes of CO_2 per tonne of ethylene, compared to 0.4 tonne of CO_2 released from the ENDP process, resulting in a 72% reduce in CO_2 emission when grid electricity is used for ENDP versus an 89% reduction when low-carbon electricity (e.g., nuclear, wind, or hydropower) is used. A 98% reduction in the carbon footprint can be achieved when low-carbon energy is used for both heat and electricity.

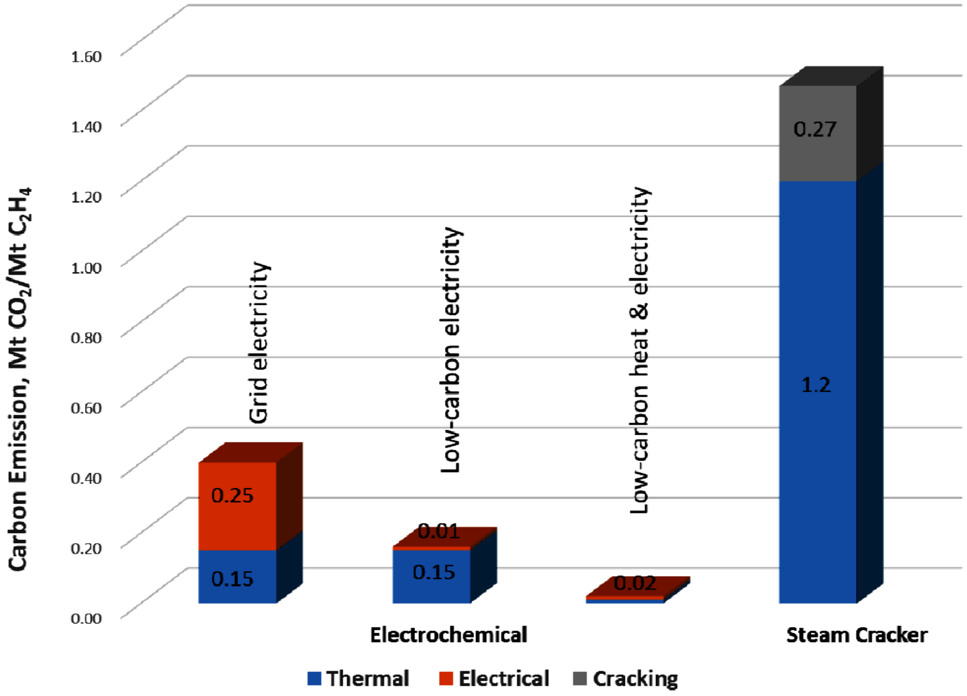

Figure 21. CO_2 emissions for ENDP and steam cracking.

4. LDPE PRODUCTION FROM ETHYLENE

The production of ethylene via ENDP has been discussed and analyzed with process and economic models in the previous sections. This next section discusses the process and economics of coupling NPP electricity and heat with the manufacture of low-density polyethylene (LDPE), using ethylene as a feedstock. Because the low-density polyethylene (LDPE) process involves much-higher pressure and temperature than other polyethylene products, such as high-density PE, LDPE is selected for ethylene utilization. Capital and operating costs were analyzed following common assumptions for polymer industries (Lack and Zanette 2001), as summarized in Table 26. All costs presented are on a 2017 constant U.S. dollar basis. The Chemical Engineering Plant Cost Index is used to convert capital and operating costs to 2017 dollars.

Table 27. Cost assumptions for LDPE production from ethylene.

Assumption description	Assumed value
Plant life	20 years
Plant financing debt/equity	60% / 40% of TCI
Interest rate for debt financing	5.0%
Term for debt financing	10 years
Construction period	3 year
On-stream factor	91% (8000 operating hours per year)
Labor	Based on plant capability
Maintenance	6% of fixed capital investment
Benefits and general overhead	50% of labor + maintenance
Administration	45% of labor
Quality control and laboratory	20% of labor
Insurance and taxes	1% of fixed capital investment
Electricity	\$0.06/kWh

The LDPE process details are based on a PE production rate of 0.83 mtpa, which is a medium-sized PE capacity for current PE plants (America Outlook 2018) and matches the ethylene-production rate from upstream. The capital and operation cost for the LDPE process are based on data from Lack and Zanette (2001). Cost estimates can be scaled to other capacities using the six-tenths factor rule [1], in which the cost of equipment scales to the 0.6 power of the capacity if the plant equipment is made larger rather than duplicated at the original scale to obtain more throughput:

$$\text{Cost of Larger System} = (\text{Original Cost}) \times (\text{Larger Capacity} / \text{Original Capacity})^{0.6}$$

Polymerization-grade ethylene is compressed to 50 bar. The on-stream time is 8,000 h/a. The tubular reactors equipped with multiple feeds of ethylene and peroxide initiators are operated at 2000 bar. The initiators are a mix of dicyclohexyl peroxy dicarbonate, t-butylperoxy pivalate, t-butylperoxy 2-ethylhexanoate, and di(t-butyl)peroxide, which are fed in past the heating zone and at two locations further downstream. The pressure of the high-pressure separator is 25 bar. A twin-screw extruder with a side extruder to process LDPE of 0.918–0.939 g/ml density and 0.3–2.0 g/10 min melt-flow index is used (Lack and Zanette 2001). The process block diagram is shown as Figure 22 below and a process-flow diagram generated from AspenPlus can be founded in Appendix B. Due to the high-pressure application of this process, nuclear power can be used for the compression system.

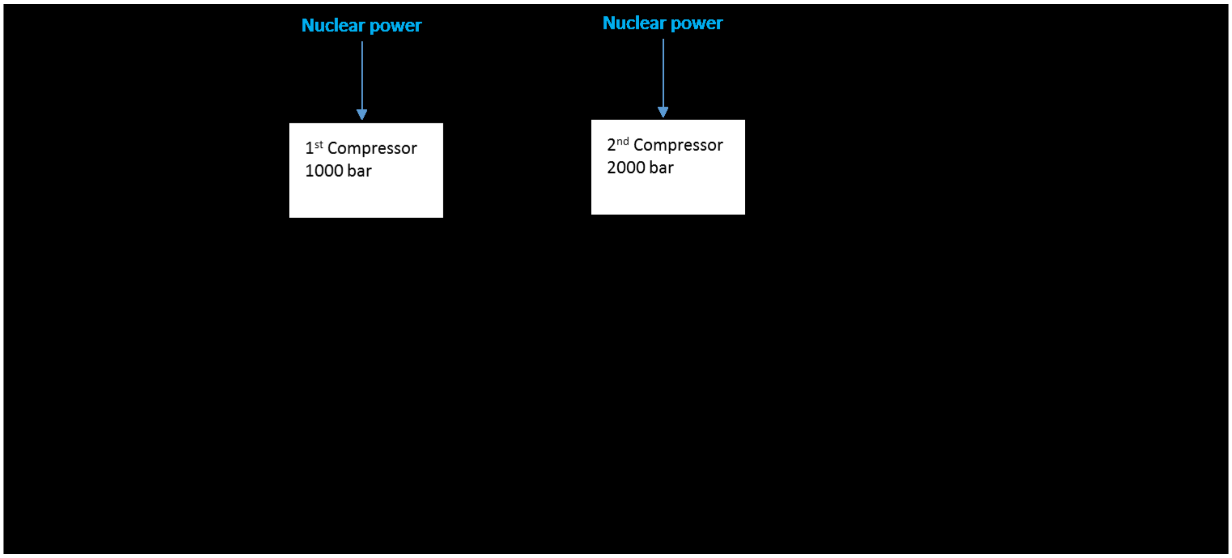

Figure 22. Process block diagram for LDPE at 830,000 tonne/year.

The capital costs of main purchased equipment are listed in Table 27 (Lack and Zanette 2001). More than 80% of the total purchased equipment costs are for the compression system, extruder, and silos. Beside purchased equipment, bulk materials, and indirect costs are required for calculating the TCI for an installed plant. Bulk materials and indirect costs, mainly include piping systems, instrumentation and control, installation, etc., are shown in Table 28. The TCI for this plant of 830,000 ton/year is about $344 million, which is four times higher than the costs of purchased equipment. This number is in agreement with the result obtained from the Lang-factor method. For liquid operation, a Lang factor of 4.74 is applied to the cost of purchased equipment for calculation of TCI (Turton 2010). Spreading the TCI over 30 years of plant life, the capital cost per year per ton of PE is about $14.

Table 28. Capital cost for LDPE process at 830,000 tonne of PE per year, on 2017 U.S. prices (in millions of dollars).

Equipment	Cost
PE reactor	4.754
Polymer separation system (including high- and low-pressure separator, was separator, recycle gas coolers)	6.656
Compression system (including primary and secondary compressor, booster compressor)	27.336
Extruder	22.106
Silo	24.008
Purchased equipment cost	84.860
Bulk materials and indirect cost	259.335
TCI w/o interest	344.195
Lang factor	4.74
TCI using Lang factor	402.236
Capital cost per metric tonne (tonne)	$415/tonne
Capital cost per metric tonne (tonne) over 20 years	$21/tonne/year

Table 29. Bulk materials and indirect cost for LDPE process.

Piping	Control and instrumentation
Installation	Coating and insulation
Traffic zone	Electrical equipment
Buildings	Remaining costs

The overall operating cost can be divided into fixed capital and variable costs. Fixed capital costs have to be taken into account when a plant is out of operation, whereas variable costs depend on the production rate. Fixed capital costs include insurance, maintenance, labor, overheads, etc. Variable costs are feedstock (ethylene), utilities, monomers, and other chemicals, such as initiators, modifiers, or stabilizers.

The specific costs were based on reference data (Lack and Zanette 2001) and were adjusted according to current situation. As presented in Table 29, the total operating costs are \$896/tonne of LDPE for a plant capacity of 830,000 tonne/year. The production costs are dominated by the cost of feedstock (ethylene), accounting for 80% of the total operating costs (Figure 23). The price of ethylene as feedstock is taken as the average price of 2017 at \$600/tonne (The pH Report 2018). Also, utilities (9%), labor (2.7%), overhead (2.5%), and maintenance (2.3%) contribute costs.

Table 30. Operating cost for LDPE process at 830,000 tonne of PE per year, on 2017 U.S. prices.

Items	**\$/tonne PE**
Ethylene (\$600/tonne)	720
Initiators (6–12 \$/kg)	5
Other chemicals	5
Electricity (\$0.06/kWh)	77
Other utilities (steam, water)	3
Insurance (1% of TCI)	3
Maintenance (6% of TCI)	21
Labor	24
Plant overhead (50% of labor and maintenance)	22
Administration (45% of labor)	11
Quality control and laboratory (20% of labor)	5
Total operation cost per metric tonne of PE	**896**
Total operation cost per metric tonne of PE w/o ethylene cost	**176**

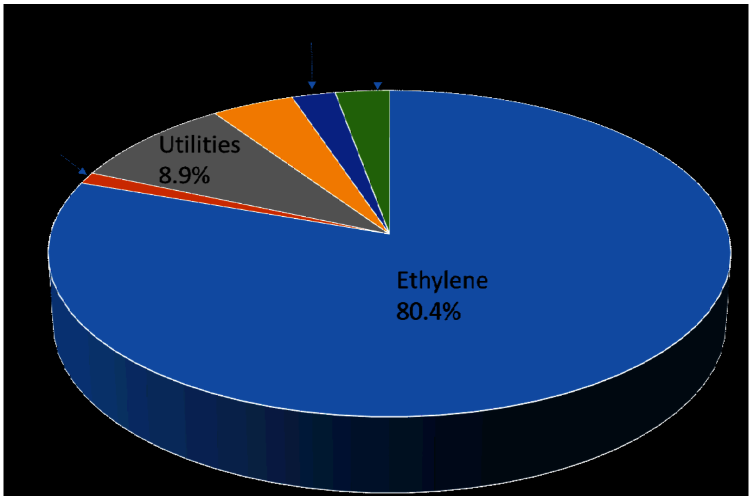

Figure 23. Composition of total operating costs (chemicals: initiators and other chemicals; utilities: electricity, steam and water; manpower: labor, administration and quality control; overhead: plant overhead and insurance).

For a conventional standalone PE plant, the LDPE results demonstrated that feedstock ethylene at a price of $600/tonne is a significantly dominant cost, contributing 80% of total operation costs. If an NPP-ENDP-PE coupled process is built, ethylene is produced onsite, resulting in much-lower ethylene prices, as the MSP of ethylene from an NPP-ENDP process is $370/tonne, as demonstrated in the Section 3. This would save the operation cost of LDPE by 40%. Therefore, this NPP-ENDP-PE coupled plant would hold promising economics compared to traditional standalone PE plants.

For LDPE production from ethane using NPP-ENDP-PE coupled process and NPP-Cracking-PE coupled process, as summarized in Table 32, The NPP-ENDP-PE process exhibits notable advantages compared to a process using traditional steam-ethane cracking in terms of capital cost (37% reduction), operating cost (16% decrease)

Table 31. Economics for LDPE production from ethane via ENDP and steam cracking processes for 830,000 tonne of PE per year, on 2017 U.S. prices.

	Unit	**ENDP**	**Cracking**
TCI	M$	760	1,525
Total operating costs (TOCs)/tonne	$/tonne PE	711	755

5. CONCLUSIONS AND RECOMMENDATIONS

For ethylene production, results demonstrate that both the nuclear-integrated ENDP current and future cases are promising compared to traditional ethane steam cracking at a similar plant size. The ENDP current case has an operating cost similar to steam cracking ($423MM vs $480MM per year), while its capital cost is 48% lower than that of steam cracking. The future case demonstrates more benefits over the steam cracking. For a typical 1 GW NPP, 420 MWe electricity, 140 MWt Steam and 25 MWt cooling duty of the NPP are required to support production of 84 metric ton per hour of ethylene with an ethane feed of 111 metric ton (tonne) per hour for the ENDP future case. These sales can provide positive revenues for the NPP. In addition, the ENDP plant also produces 7 tonne/hour of hydrogen and a stream of 20 tonne/hour of other C3 to C4 hydrocarbons which can be sold as a co-product stream. Substituting nuclear power and heat in lieu of natural gas for heats of ENDP reaction requirements results in a over 70% CO2 emission reduction. On the other hand, the steam cracking produces 94 tonne ethylene per hour; however its energy requirement per tonne ethylene produced is 37% higher than that of the ENDP future process.

Economically, the nuclear-integrated ENDP future case shows potential higher profitability than the conventional steam cracking plant. The ENDP CAPEX ($345M) and OPEX ($395M/year) are 68% and 7% lower than that of steam cracking, respectively. With an IRR of 12%, the MSP of produced ethylene is $0.37/kg for ENDP, which is 48% lower than that of steam cracking ($0.71/kg). The MSP of steam cracking is lower than that of current market ethylene price ($0.44/kg). With an IRR of 12% and a selling price of ethylene at $0.44/kg ($0.2/lb), the anticipated NPV for the ENDP future plant is $285M and the DPBP is five years of operation. It is worth noting that the current industrial ethylene price is at $0.44/kg ($0.2/lbs) is almost history record low price.

Among the many factors affecting the final price of produced ethylene, the price of feedstock ethane is the biggest influencer, causing 35% variation on the MSP of produced ethylene from every $0.1/kg change of ethane, followed by the prices of electricity, hydrogen and propylene.

In summary, the nuclear-integrated ENDP future case exhibits several possible advantages over traditional steam cracking, including a 68% reduction in capital costs, a 7% decrease in operating costs, and a more than 70% reduction in carbon footprint. In addition, its economic performance is promising by achieving an NPV of $285M at a selling price of $0.44/kg and an IRR of 12%.

From the results obtained in this study, the following items and recommendation are listed for to be performed in the future to further refine the process and economic modeling of the ENDP process:

- Three areas are targeted for research and improvement in order to achieve ENDP future case—i.e., ethylene single-pass yield of 48.5%. These areas are electrocatalysts, cell component materials, and overall process optimization.
  - *Development of Electrocatalysts*: Novel electrocatalysts that can maximize the benefits of electrochemistry by efficiently enabling the flow of electrons, while also enabling the desired reactions. By so doing, "true" electrocatalysis and high conversion can be realized of ethane at reduced temperatures where side reactions, catalyst deactivation and coking will be remarkably suppressed.
  - *Cell Component Materials*: One of the technical opportunities is to improve the proton-transference number of the electrolyte and the resulting Faradaic efficiency in a reducing atmosphere. This will allow the electrochemical cell to operate at much-higher current densities with sufficient proton flux. The benefits include not only faster driving force to move the reaction forward, but larger quantities of hydrogen produced at the cathode side, as well as distinctly reduced separation cost when co-occurrent hydrogen at the anode side is too hard to separate.
  - *Overall Process Optimization*: In addition to the development of the materials and catalysts,

it is crucial to investigate the effects of all operating conditions on the ultimate yield of ethylene and lifetime durability. Specific design of the electrochemical cell and stack, scale and modularity, as well as engineering of feedstock and downstream distribution, are important factors for achieving an economically viable operation. It is expected that an effective combination of experiments, modeling, and technoeconomic analyses is the key for the further development and implementation of ENDP to meet the projected targets, which are attainable.

- The ENDP reactor is the core for the plant. Alternative methods to estimate the capital cost, operating and manufacturing costs, energy requirement should be developed to refine the economic results. For the ENDP future case in this study, the ENDP capital cost is obtained using H2A model for hydrogen production from SOEC using a stack capital of $150/kW, and a 20% safety margin is used. First, this number is higher than other studies on SOECs. Second, this method might not be accurate to estimate the capital cost of the ENDP reactor. A bottom-up method may be a good route for capital-cost estimation.

- The ENDP reactor design for commercial scale needs rigorous investigation in the future, including the an analysis of the networking system within each individual stack, the control-valve system, and stack replacement, etc. An electrical system is employed in this study for providing reaction heat. The feasibility and safety of this heating system is worth further consideration.

- Efficiency and capital cost of membrane systems used in this study need further investigation to reduce the energy and cost requirements. An amount of $50M is used as the capital cost of the membrane system for ethane and ethylene separation, which is almost four times higher than those used in distillation systems while the membrane system is supposed to be a simpler and more highly energy efficient system than those employed in distillation columns.

- The simplified COLDBOX unit for refrigeration should be replaced with more rigorous models based on actual operation input to refine its CAPEX and OPEX.

- Heat- and material-integration techniques can be applied to identify areas that can be pinched to reduce the minimum heating and cooling requirements, thereby reducing energy consumption and also the number of equipment.

A separate study should be conducted on the method of integration of an ENDP plant with an NPP to assess the optimal siting, balancing safety concerns associated with separation distance and heat losses associated with transporting high-temperature heat long distances.

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Appendix A

Process-Flow Diagrams

Appendix A

Process-Flow Diagrams

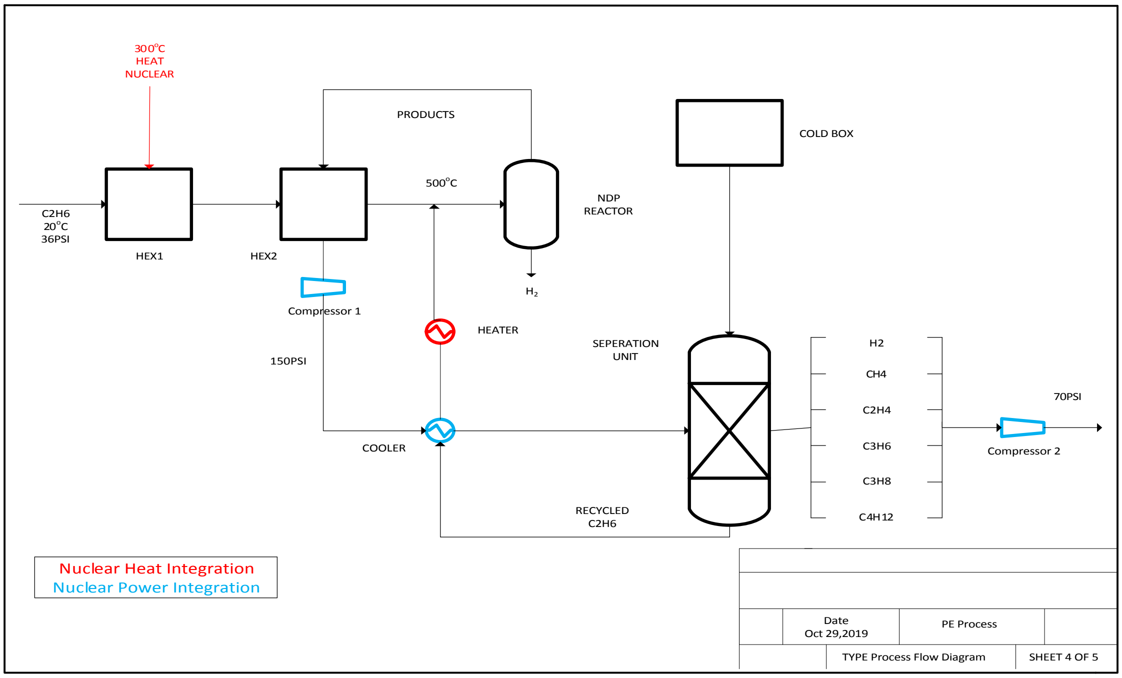

Table A- 1. Block flow diagram for ethylene production from ENDP process.

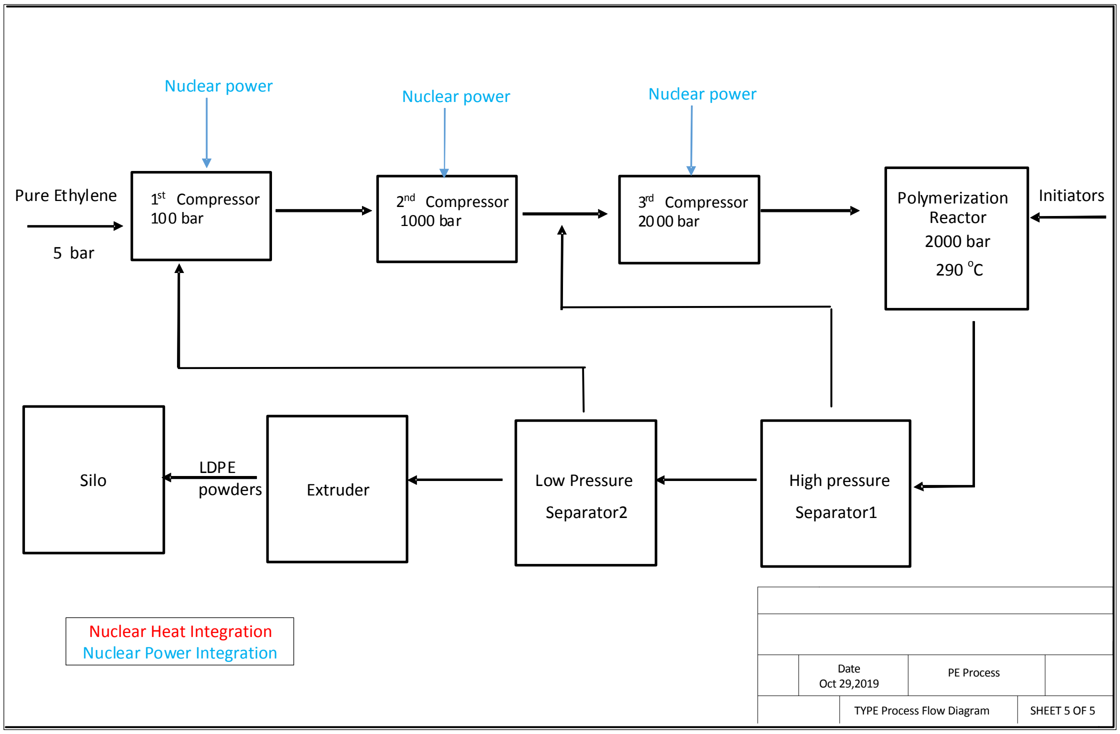

Table A- 2. Block flow diagram for LDPE production.

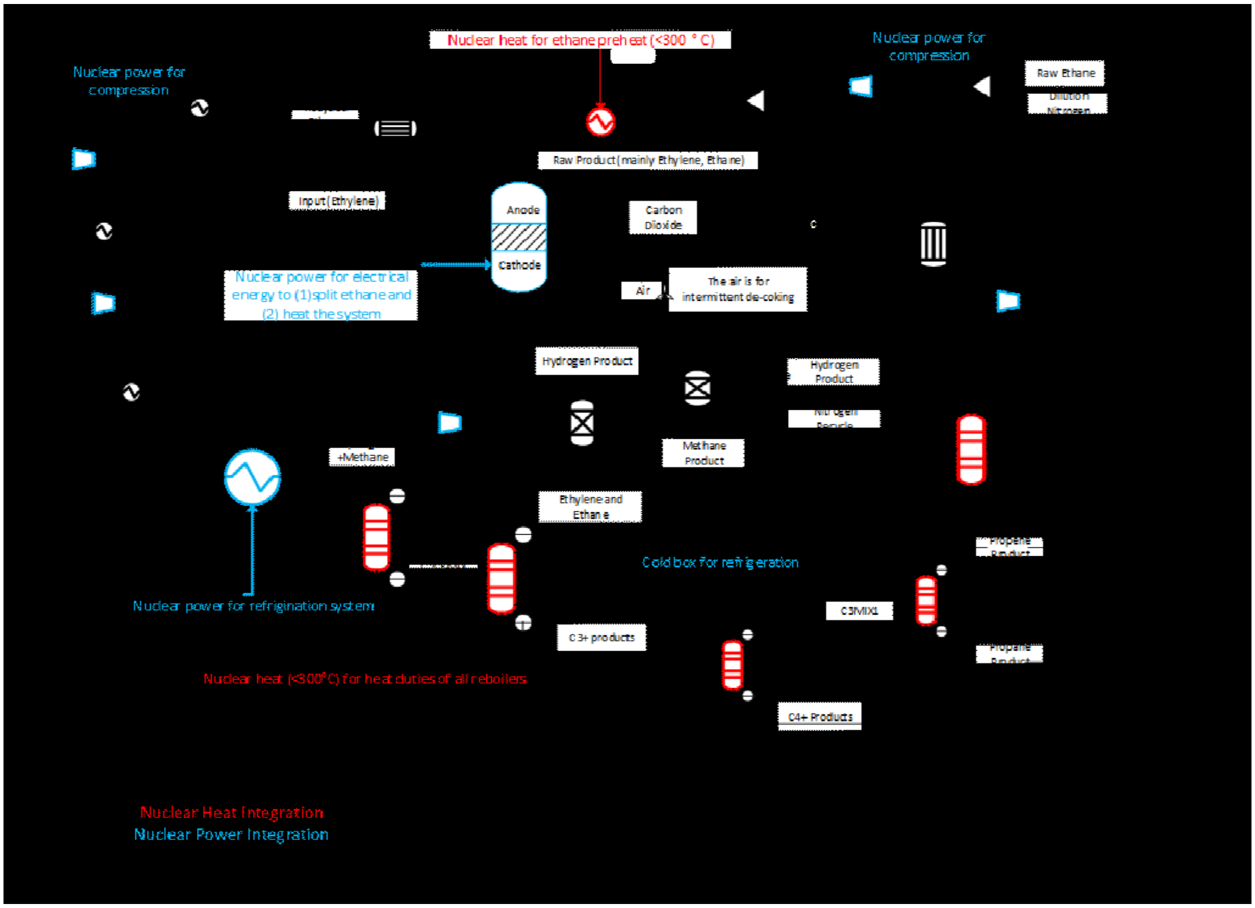

Table A- 3. Process-flow diagram for ethylene production from ENDP process.

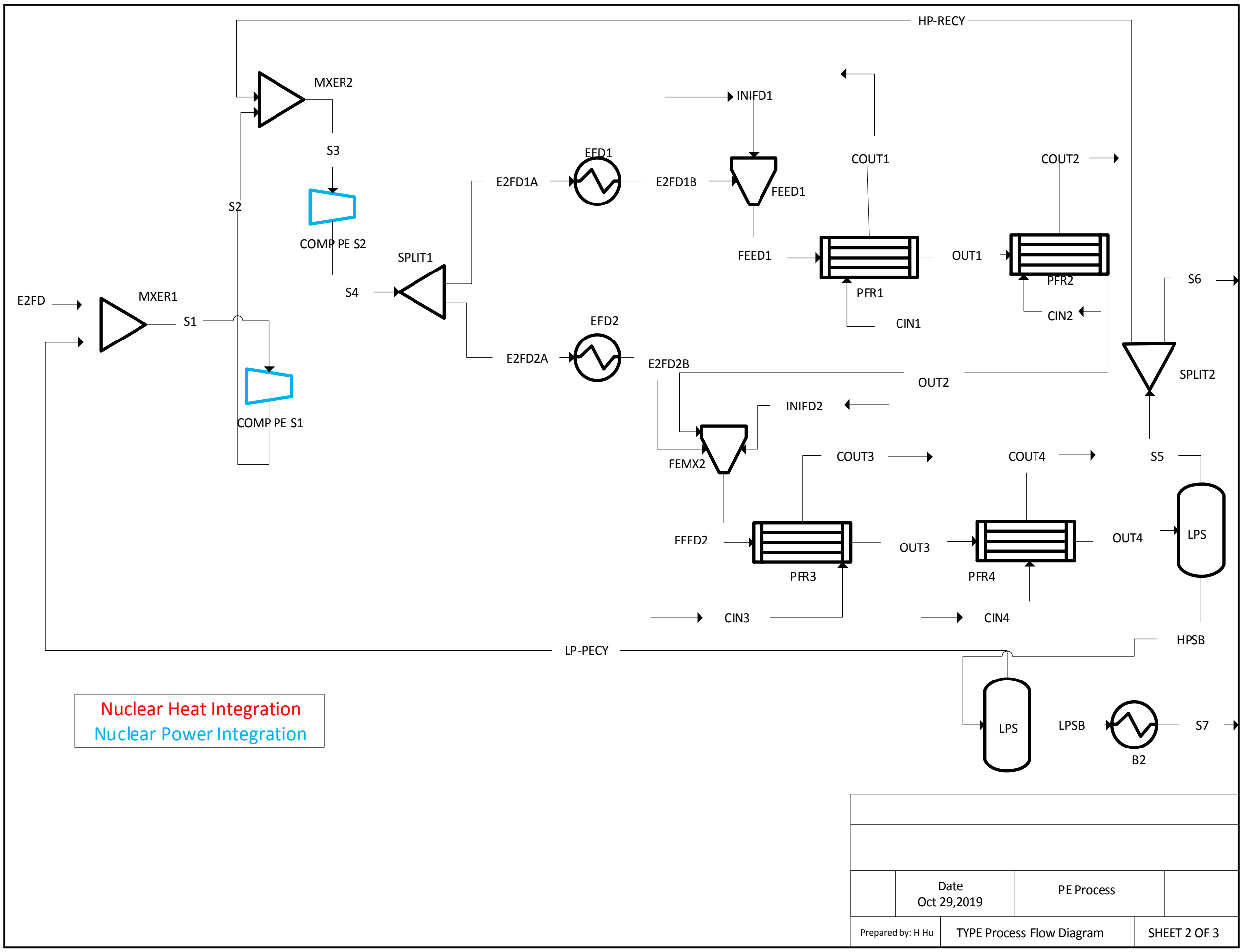

Table A- 4. Process-flow diagram for LDPE production.

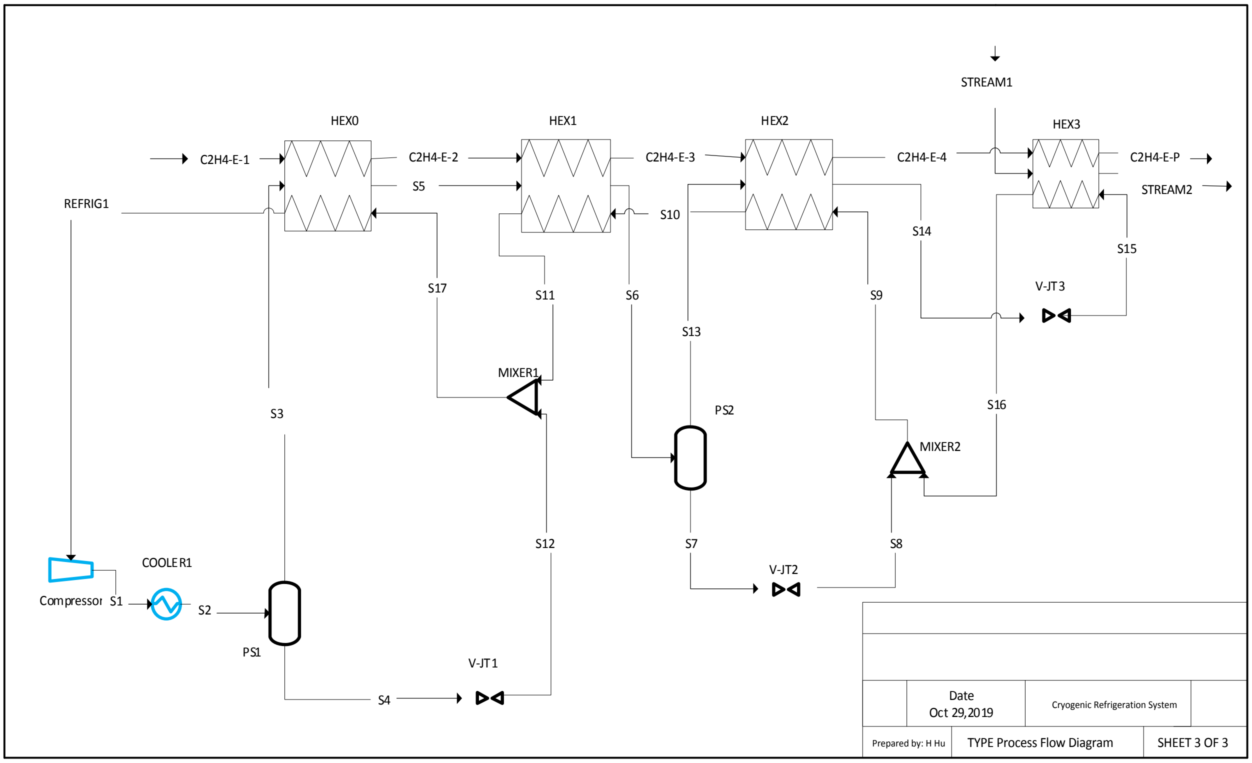

Table A- 5. Process-flow diagram for refrigeration system for the ENDP and PE process.

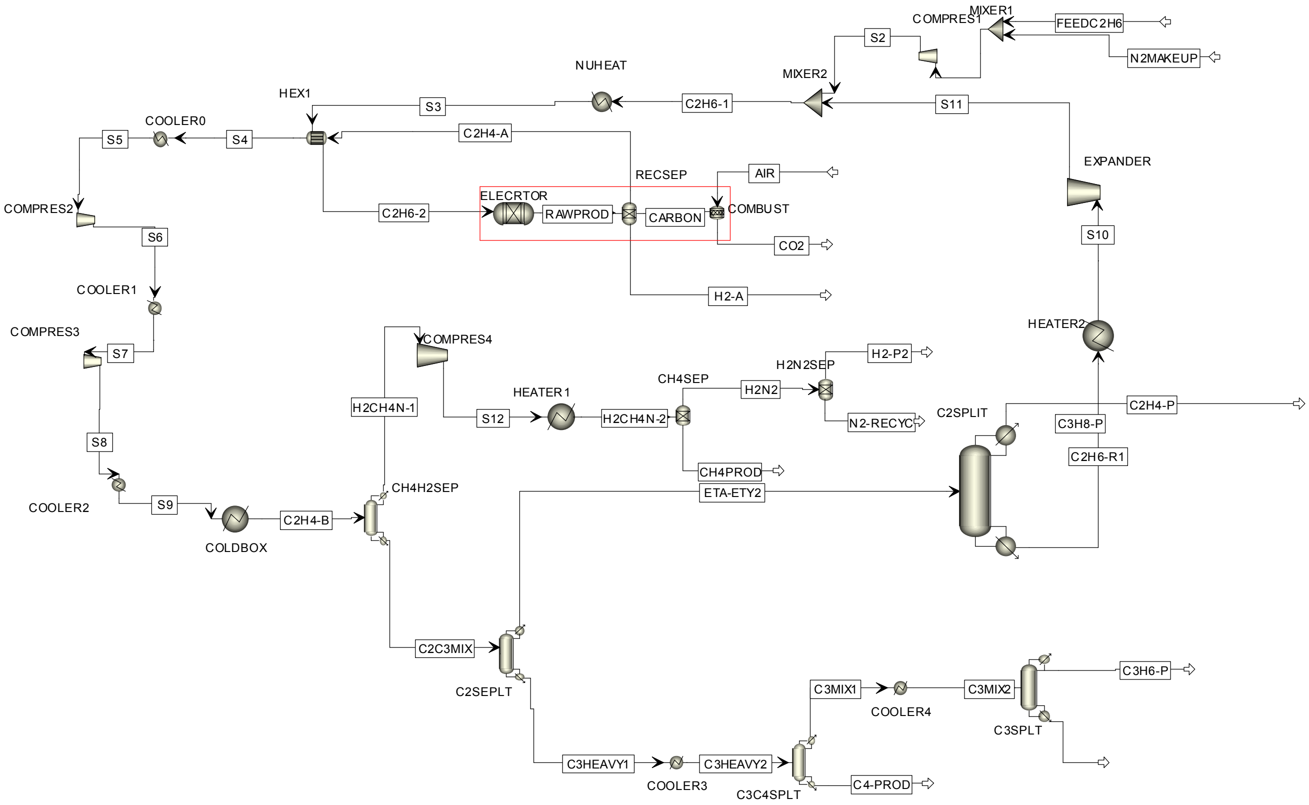

Table A- 6. AspenPlus simulation for ethylene production from the ENDP current case process (objects inside the red dashed line are one piece in reality).

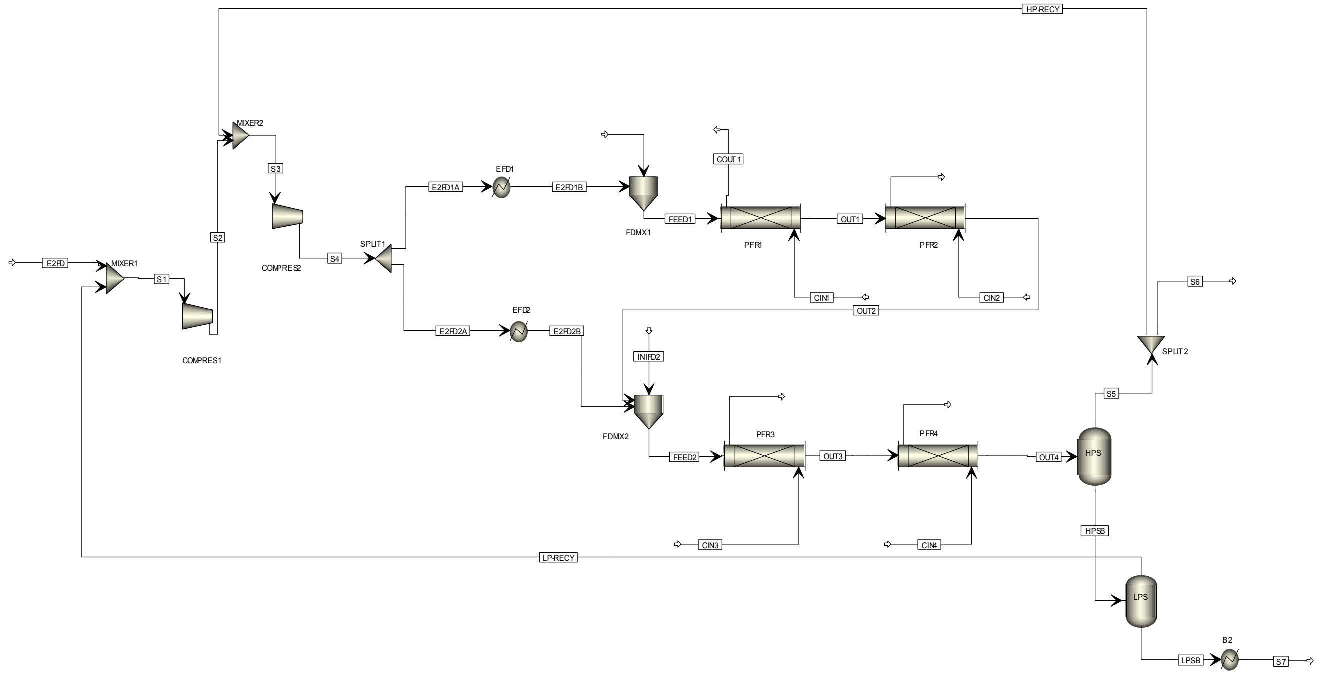

Table A- 7. AspenPlus simulation for LDPE production.

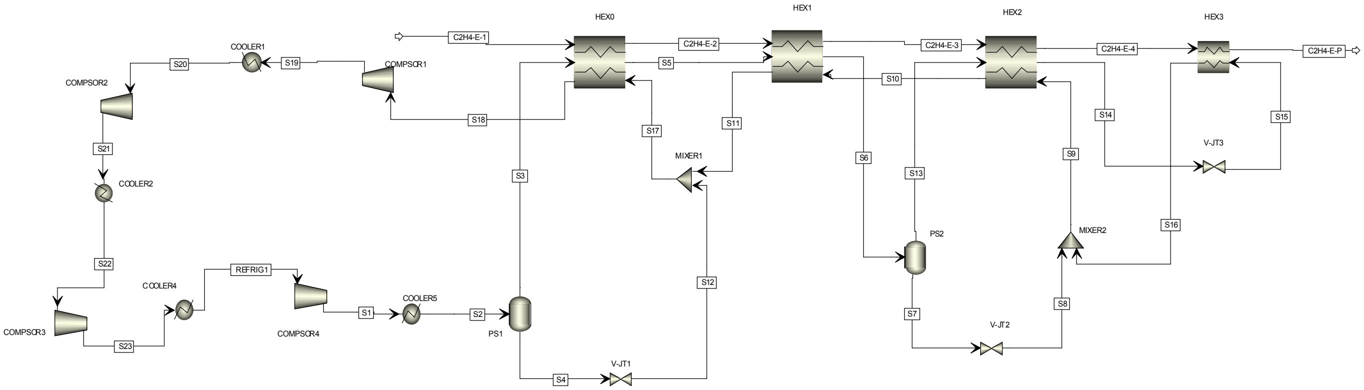

Table A- 8. AspenPlus simulation for cryogenic refrigeration system for the ENDP and PE process.

Appendix B

Process Mass Balance for ENDP

Appendix B

Process mass balance for ENDP

Table B- 1. Mass balance for all the streams for the ENDP current process simulated by AspenPlus.

	Units	C2C3MIX	C2H4-A	C2H4-B	C2H4-P	C2H6-1	C2H6-2
ETHANE	kg/hr	177368.63	177368.69	177368.69	44.71	288289.86	288289.86
OXYGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE	kg/hr	73351.22	73352.89	73352.89	72571.75	779.20	779.20
HYDROGEN	kg/hr	0.00	3577.93	3577.93	0.00	0.00	0.00
NITROGEN	kg/hr	0.00	37000.00	37000.00	0.00	37000.00	37000.00
METHANE	kg/hr	0.99	2200.80	2200.80	0.99	0.00	0.00
1-BUT-01	kg/hr	22634.92	22634.92	22634.92	0.00	0.00	0.00
PROPANE	kg/hr	538.69	538.69	538.69	0.00	0.40	0.40
PROPY-01	kg/hr	5738.68	5738.68	5738.68	0.00	45.09	45.09
CARBON	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flows	kg/hr	279633.13	322412.61	322412.61	72617.45	326114.56	326114.56
Mole Fractions							
ETHANE		0.65	0.48	0.48	0.00	0.88	0.88
OXYGEN		0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE		0.29	0.21	0.21	1.00	0.00	0.00
HYDROGEN		0.00	0.14	0.14	0.00	0.00	0.00
NITROGEN		0.00	0.11	0.11	0.00	0.12	0.12
METHANE		0.00	0.01	0.01	0.00	0.00	0.00
1-BUT-01		0.04	0.03	0.03	0.00	0.00	0.00
PROPANE		0.00	0.00	0.00	0.00	0.00	0.00
PROPY-01		0.02	0.01	0.01	0.00	0.00	0.00
CARBON		0.00	0.00	0.00	0.00	0.00	0.00
CO2		0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	lbmol/hr	19985.64	27112.85	27112.85	5706.51	24112.08	24112.08
Temperature	C	-37.80	550.00	-150.00	-59.79	6.65	537.41
Pressure	psia	144.00	30.00	145.00	110.00	36.00	33.00
Molar Vapor Fraction		0.00	1.00	0.23	1.00	1.00	1.00
Molar Liquid Fraction		1.00	0.00	0.77	0.00	0.00	0.00
Average MW		30.85	26.22	26.22	28.05	29.82	29.82

Table B- 1. continued

	Units	C2H6-R1	C3H6-P	C3H8-P	C3HEAVY 1	C3HEAVY 2	C3MIX1
ETHANE	kg/hr	177289.86	34.06	0.00	34.06	34.06	34.06
OXYGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE	kg/hr	779.20	0.27	0.00	0.27	0.27	0.27
HYDROGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
NITROGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
METHANE	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
1-BUT-01	kg/hr	0.00	0.00	284.60	22634.92	22634.92	284.60
PROPANE	kg/hr	0.40	220.84	277.20	538.29	538.29	498.04
PROPY-01	kg/hr	45.09	5149.37	369.18	5693.59	5693.59	5518.55
CARBON	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flows	kg/hr	178114.56	5404.54	930.98	28901.13	28901.13	6335.52
Mole Fractions							
ETHANE		1.00	0.01	0.00	0.00	0.00	0.01
OXYGEN		0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE		0.00	0.00	0.00	0.00	0.00	0.00
HYDROGEN		0.00	0.00	0.00	0.00	0.00	0.00
NITROGEN		0.00	0.00	0.00	0.00	0.00	0.00
METHANE		0.00	0.00	0.00	0.00	0.00	0.00
1-BUT-01		0.00	0.00	0.25	0.73	0.73	0.03
PROPANE		0.00	0.04	0.31	0.02	0.02	0.08
PROPY-01		0.00	0.95	0.44	0.25	0.25	0.88
CARBON		0.00	0.00	0.00	0.00	0.00	0.00
CO2		0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	lbmol/hr	13062.02	283.34	44.38	1217.11	1217.11	327.72
Temperature	C	-35.75	11.60	26.35	52.31	1.00	18.75
Pressure	psia	130.00	120.00	130.00	144.00	139.00	130.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	1.00
Molar Liquid Fraction		1.00	1.00	1.00	1.00	1.00	0.00
Average MW		30.06	42.05	46.24	52.35	52.35	42.62

Table B- 1. continued

	Units	C3MIX2	C4-PROD	CARBON	CH4PROD	CO2	ETA-ETY2
ETHANE	kg/hr	34.06	0.00	0.00	0.07	0.00	177334.57
OXYGEN	kg/hr	0.00	0.00	0.00	0.00	14184.00	0.00
ETHYLENE	kg/hr	0.27	0.00	0.00	1.67	0.00	73350.96
HYDROGEN	kg/hr	0.00	0.00	0.00	178.90	0.00	0.00
NITROGEN	kg/hr	0.00	0.00	0.00	370.00	0.00	0.00
METHANE	kg/hr	0.00	0.00	0.00	2197.61	0.00	0.99
1-BUT-01	kg/hr	284.60	22350.32	0.00	0.00	0.00	0.00
PROPANE	kg/hr	498.04	40.25	0.00	0.00	0.00	0.40
PROPY-01	kg/hr	5518.55	175.04	0.00	0.00	0.00	45.09
CARBON	kg/hr	0.00	0.00	124.02	0.00	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00	0.00	454.43	0.00
Total Mass Flows	kg/hr	6335.52	22565.61	124.02	2748.24	14638.43	250732.00
Mole Fractions							
ETHANE		0.01	0.00	0.00	0.00	0.00	0.69
OXYGEN		0.00	0.00	0.00	0.00	0.98	0.00
ETHYLENE		0.00	0.00	0.00	0.00	0.00	0.31
HYDROGEN		0.00	0.00	0.00	0.37	0.00	0.00
NITROGEN		0.00	0.00	0.00	0.06	0.00	0.00
METHANE		0.00	0.00	0.00	0.57	0.00	0.00
1-BUT-01		0.03	0.99	0.00	0.00	0.00	0.00
PROPANE		0.08	0.00	0.00	0.00	0.00	0.00
PROPY-01		0.88	0.01	0.00	0.00	0.00	0.00
CARBON		0.00	0.00	1.00	0.00	0.00	0.00
CO2		0.00	0.00	0.00	0.00	0.02	0.00
Mole Flows	lbmol/hr	327.72	889.39	22.76	526.90	1000.00	18768.53
Temperature	C	1.00	69.17	550.00	20.00	500.00	-40.91
Pressure	psia	130.00	140.00	30.00	1000.00	30.00	130.00
Molar Vapor Fraction		0.00	0.00	0.00	1.00	1.00	1.00
Molar Liquid Fraction		1.00	1.00	1.00	0.00	0.00	0.00
Average MW		42.62	55.94	12.01	11.50	32.27	29.45

Table B- 1. continued

	Units	FEEDC2H6	H2-A	H2-P2	H2CH4N-1	H2CH4N-2	H2N2
ETHANE	kg/hr	111000.00	0.00	0.00	0.07	0.07	0.00
OXYGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE	kg/hr	0.00	0.00	0.00	1.67	1.67	0.00
HYDROGEN	kg/hr	0.00	3577.93	3229.08	3577.93	3577.93	3399.03
NITROGEN	kg/hr	0.00	0.00	366.30	37000.00	37000.00	36630.00
METHANE	kg/hr	0.00	0.00	0.00	2199.81	2199.81	2.20
1-BUT-01	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
PROPANE	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
PROPY-01	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
CARBON	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flows	kg/hr	111000.00	3577.93	3595.38	42779.47	42779.47	40031.23
Mole Fractions							
ETHANE		1.00	0.00	0.00	0.00	0.00	0.00
OXYGEN		0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE		0.00	0.00	0.00	0.00	0.00	0.00
HYDROGEN		0.00	1.00	0.99	0.55	0.55	0.56
NITROGEN		0.00	0.00	0.01	0.41	0.41	0.44
METHANE		0.00	0.00	0.00	0.04	0.04	0.00
1-BUT-01		0.00	0.00	0.00	0.00	0.00	0.00
PROPANE		0.00	0.00	0.00	0.00	0.00	0.00
PROPY-01		0.00	0.00	0.00	0.00	0.00	0.00
CARBON		0.00	0.00	0.00	0.00	0.00	0.00
CO2		0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	lbmol/hr	8138.21	3912.92	3560.24	7127.21	7127.21	6600.31
Temperature	C	20.00	550.00	20.00	-171.25	20.00	20.00
Pressure	psia	20.00	30.00	80.00	135.00	1000.00	80.00
Molar Vapor Fraction		1.00	1.00	1.00	1.00	1.00	1.00
Molar Liquid Fraction		0.00	0.00	0.00	0.00	0.00	0.00

Average MW		30.07	2.02	2.23	13.23	13.23	13.37

Table B- 1. continued

	Units	**N2-RECYC**	**N2MAKEUP**	**RAWPROD**	**S1**	**S2**	**S3**
ETHANE	kg/hr	0.00	0.00	177368.69	111000.00	111000.00	288289.86
OXYGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE	kg/hr	0.00	0.00	73352.89	0.00	0.00	779.20
HYDROGEN	kg/hr	169.95	0.00	7155.86	0.00	0.00	0.00
NITROGEN	kg/hr	36263.70	37000.00	37000.00	37000.00	37000.00	37000.00
METHANE	kg/hr	2.20	0.00	2200.80	0.00	0.00	0.00
1-BUT-01	kg/hr	0.00	0.00	22634.92	0.00	0.00	0.00
PROPANE	kg/hr	0.00	0.00	538.69	0.00	0.00	0.40
PROPY-01	kg/hr	0.00	0.00	5738.68	0.00	0.00	45.09
CARBON	kg/hr	0.00	0.00	124.02	0.00	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flows	kg/hr	36435.85	37000.00	326114.56	148000.00	148000.00	326114.56
Mole Fractions							
ETHANE		0.00	0.00	0.42	0.74	0.74	0.88
OXYGEN		0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE		0.00	0.00	0.19	0.00	0.00	0.00
HYDROGEN		0.06	0.00	0.25	0.00	0.00	0.00
NITROGEN		0.94	1.00	0.09	0.26	0.26	0.12
METHANE		0.00	0.00	0.01	0.00	0.00	0.00
1-BUT-01		0.00	0.00	0.03	0.00	0.00	0.00
PROPANE		0.00	0.00	0.00	0.00	0.00	0.00
PROPY-01		0.00	0.00	0.01	0.00	0.00	0.00
CARBON		0.00	0.00	0.00	0.00	0.00	0.00
CO2		0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	lbmol/hr	3040.07	2911.85	31048.54	11050.06	11050.06	24112.08
Temperature	C	20.00	20.00	550.00	19.85	63.78	265.00
Pressure	psia	80.00	20.00	30.00	20.00	36.00	36.00
Molar Vapor							

Fraction							
Molar Liquid Fraction		0.00	0.00	0.00	0.00	0.00	0.00
Average MW		26.42	28.01	23.16	29.53	29.53	29.82

Table B- 1. continued

	Units	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**
ETHANE	kg/hr	177368.69	177368.69	177368.69	177368.69	177368.69	177368.69
OXYGEN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE	kg/hr	73352.89	73352.89	73352.89	73352.89	73352.89	73352.89
HYDROGEN	kg/hr	3577.93	3577.93	3577.93	3577.93	3577.93	3577.93
NITROGEN	kg/hr	37000.00	37000.00	37000.00	37000.00	37000.00	37000.00
METHANE	kg/hr	2200.80	2200.80	2200.80	2200.80	2200.80	2200.80
1-BUT-01	kg/hr	22634.92	22634.92	22634.92	22634.92	22634.92	22634.92
PROPANE	kg/hr	538.69	538.69	538.69	538.69	538.69	538.69
PROPY-01	kg/hr	5738.68	5738.68	5738.68	5738.68	5738.68	5738.68
CARBON	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flows	kg/hr	322412.61	322412.61	322412.61	322412.61	322412.61	322412.61
Mole Fractions							
ETHANE		0.48	0.48	0.48	0.48	0.48	0.48
OXYGEN		0.00	0.00	0.00	0.00	0.00	0.00
ETHYLENE		0.21	0.21	0.21	0.21	0.21	0.21
HYDROGEN		0.14	0.14	0.14	0.14	0.14	0.14
NITROGEN		0.11	0.11	0.11	0.11	0.11	0.11
METHANE		0.01	0.01	0.01	0.01	0.01	0.01
1-BUT-01		0.03	0.03	0.03	0.03	0.03	0.03
PROPANE		0.00	0.00	0.00	0.00	0.00	0.00
PROPY-01		0.01	0.01	0.01	0.01	0.01	0.01
CARBON		0.00	0.00	0.00	0.00	0.00	0.00
CO2		0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	lbmol/hr	27112.85	27112.85	27112.85	27112.85	27112.85	27112.85

Temperature	C	275.00	1.00	88.06	1.00	47.91	1.00
Pressure	psia	25.00	25.00	80.00	80.00	150.00	150.00
Molar Vapor Fraction		1.00	1.00	1.00	1.00	1.00	1.00
Molar Liquid Fraction		0.00	0.00	0.00	0.00	0.00	0.00
Average MW		26.22	26.22	26.22	26.22	26.22	26.22

Table B- 1. continued

	Units	**S10**	**S11**	**S12**
ETHANE	kg/hr	177289.86	177289.86	0.07
OXYGEN	kg/hr	0.00	0.00	0.00
ETHYLENE	kg/hr	779.20	779.20	1.67
HYDROGEN	kg/hr	0.00	0.00	3577.93
NITROGEN	kg/hr	0.00	0.00	37000.00
METHANE	kg/hr	0.00	0.00	2199.81
1-BUT-01	kg/hr	0.00	0.00	0.00
PROPANE	kg/hr	0.40	0.40	0.00
PROPY-01	kg/hr	45.09	45.09	0.00
CARBON	kg/hr	0.00	0.00	0.00
CO2	kg/hr	0.00	0.00	0.00
Total Mass Flows	kg/hr	178114.56	178114.56	42779.47
Mole Fractions				
ETHANE		1.00	1.00	0.00
OXYGEN		0.00	0.00	0.00
ETHYLENE		0.00	0.00	0.00
HYDROGEN		0.00	0.00	0.55
NITROGEN		0.00	0.00	0.41
METHANE		0.00	0.00	0.04
1-BUT-01		0.00	0.00	0.00
PROPANE		0.00	0.00	0.00
PROPY-01		0.00	0.00	0.00
CARBON		0.00	0.00	0.00
CO2		0.00	0.00	0.00
Mole Flows	lbmol/hr	13062.02	13062.02	7127.21

Temperature	C	5.00	-39.79	-59.81
Pressure	psia	130.00	36.00	1000.00
Molar Vapor Fraction		1.00	1.00	1.00
Molar Liquid Fraction		0.00	0.00	0.00
Average MW		30.06	30.06	13.23

Appendix C

ENDP Reactor Design

Appendix C

ENDP Reactor Design

C1. THEORETICAL TOTAL ENERGY DEMAND FOR THE ENDP REACTOR

For ethylene production from ethane dissociation:

$$C_2H_6 = C_2H_4 + H_2$$

$$\Delta H_r$$

The total energy demand, ΔH_r, includes thermal energy, ΔQ, and electrical energy, which is equal to the negative of the Gibbs free-energy change, ΔG, as following equation

$$\Delta H_r = \Delta Q + \Delta G = T\Delta S + \Delta G \qquad \text{(Eq. C1)}$$

As reported for hydrogen production from HTE, the Gibbs free-energy change, ΔG_R, for the reacting system decreases with increasing temperature while the product of temperature and the entropy change, $T\Delta S_R$, increases as demonstrated in Figure C- 1. Therefore, for reversible operation, the electrical work requirement decreases with temperature, and a larger fraction of the total energy required for electrolysis, ΔH_R, can be supplied in the form of heat (O'Brien 2008).

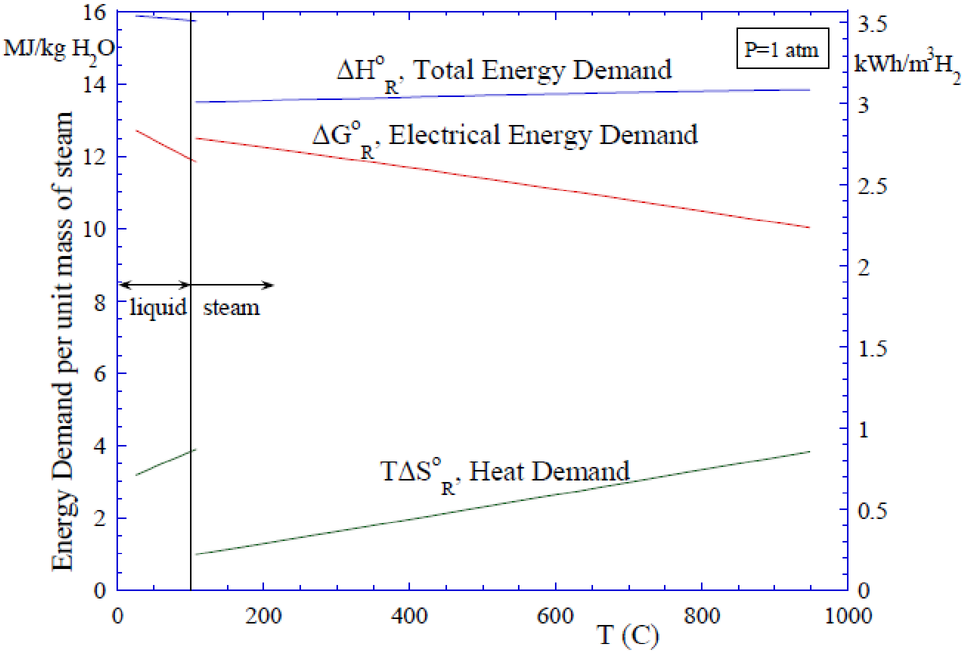

Figure C- 1. Standard-state energy requirements for electrolysis as a function of temperature (Adapted from O'Brien 2008)

C2. THEORETICAL THERMAL ENERGY REQUIRED FOR THE ENDP REACTOR AT 500°C

Assuming a temperature of 525 °C (798.15 K), entropy of 139.32 J/mol-K, and molecular weight for ethylene of 28gm/mol, the heat required can be calculated as:

$$\Delta Q = T\,\Delta S = 798.15\ (K) \times 139.32\ J/mol\text{-}K = 3.97\ GJ/tonne\ C2H4$$

This thermal energy requirement can be obtained by burning natural gas, or it can be provided using electrical heating equipment.

C3. THEORETICAL ELECTRICAL ENERGY REQUIRED FOR THE ENDP REACTOR

In this study, the current density for the ENDP process is 40mA/cm^2, corresponding to 0.09 VDC applied to the cell (V_{app}). The required electrical energy to produce C_2H_4 is thus

$0.09\ (V) \times 2\ (e) \times 6.022 \times 10^{23}/mol\ C_2H_4 = 1.1 \times 10^{23}\ eV/mol\ C_2H_4 = 17.7\ kJ/mol = 0.63\ GJ/tonne$

Therefore, the total energy demand is $\Delta H = 3.97 + 0.63 = 4.6$ GJ/tonne ethylene.

The duty requirement calculated from AspenPlus simulation is the ΔH, which includes both the required thermal energy and electrical energy. The ΔH = 419 MMBTU/hr for a flow rate of ethylene of 54.45 tonnes/hr, i.e., 7.8 GJ/tonne ethylene, which is higher than that of theoretical number (4.6 GJ/tonne). Several factors attribute to the difference: (1) there are six reactions simulation in the AspenPlus simulation for the ENDP reactor as shown in Table C- 1, while only one reaction is considered for the theoretical calculation; (2) the temperature difference between input (494 ℃) and reaction (500℃).

Area-specific resistance (ASR) represents the net effects of all the loss mechanisms in the electrolysis stack including ohmic losses, activation, and concentration overpotential, etc. (O'Brien 2008) and is applied for this ENDP reactor to account potential electricity requirement. An average ASR of 0.544 Ohm-cm^2 is reported for an HTE system (Krull et al. 2013). Therefore, the additional required voltage is :

$V_{ASR} = I \times ASR = 0.04\ A/cm^2) \times 0.544\ Ohm\text{-}cm^2 = 0.022\ V.$

So, the theoretically required applied voltage : $V_{theo} = V_{ASR} + V_{app} = 0.022 + 0.09 = 0.112$ V.

If a safety factor of 1.2 is applied (Turton et al. 2010), the overall required applied voltage:

$V_{total} = 1.2 \times 0.112 = 0.1344$ V

Correspondingly, the **required electricity energy** is:

$E = 0.1344\ (V) \times 2\ (e) \times 6.022 \times 10^{23}/mol\ C2H4 = 1.65 \times 10^{23}\ eV/mol\ C2H4 = 26.4\ kJ/mol = 0.94$ GJ/tonne

Then, the required thermal energy is:

Q = 7.8 – 0.94 = 6.86 GJ/tonne ethylene.

C4. THEORETICAL ELECTRICAL ENERGY REQUIRED FOR THE ENDP REACTOR

The reaction itself has no CO_2 released, the CO_2 comes from two section: one with fuel burn for heating the reactor to provide the heat requirement, another one is electricity requirement for the reactor.

Briefly, the heat requirement for the ENDP reaction : $Q = 89.7\ kJ/mole\text{-}C_2H_4 = 0.025\ kWh/mol\text{-}C_2H_4$

The electricity requirement for the ENDP reaction : $E = 0.021\ kWh/mol\text{-}C_2H_4$

So, if burning natural gas for the heat, the CO_2 released by burning is: 0.15 tonne CO2/tonne ethylene.

If using traditional power (whose grid electricity has a carbon intensity of 320 g CO2/kWh), the CO2 emission is; 0.15 tonne CO2/tonne ethylene.

If using renewable power (such as wind, hydro, or nuclear), their grid electricity has a carbon intensity of 18 g-CO_2/kWh, so, the CO_2 emission is 0.01 tonne CO2/tonne ethylene for both heat and electricity requirement.

C5. EFFECTS OF FEED COMPOSITION AND POSSIBLE REACTORS IN SERIAL

Because the single-pass ethylene yield for the current case is low, (less than 25% for all temperature tested, 400 – 550 °C), reactors in serial was explored as an option to increase ethane conversion and ethylene yield. However, considering the species which are more reactive than ethane (such as ethylene, C_{3+}, etc) present in the ENDP reactor anode side, preliminary experiments showed that ethylene yield decreased due to side reactions converting ethylene product into undesirable products.

C6. Theoretical Capital Cost for the ENDP Reactor

Cost for single cell, stack and modular:

1. Single cell : Figure 1 and Table 1
2. Stack cells: Figure 2 and Table 2.
3. Module : Table 3

Table C- 1. 1-in. diameter cell composition and cost.

Items	**Value**	**Unit**
Anode:		
Anode and electrolyte diameter	1	inch
Anode thickness	450	µm
Anode porosity	34%	
BZCYYb density	6.211	g*cm^{-3}
NiO density	6.67	g*cm^{-3}
Electrolyte:		
Electrolyte thinkness	10	µm
Electrolyte porosity	3%	
BZCYYb density	6.211	g*cm^{-3}
Cathode:		
Cathode diameter	0.5	Inch
Cathode thickness	30	Um
Cathode porosity	34%	
PBSCF density	6.2	g*cm^{-3}

Total material cost:	0.5	$/piece
Manufacturing cost:		
Total cost of one cell:		

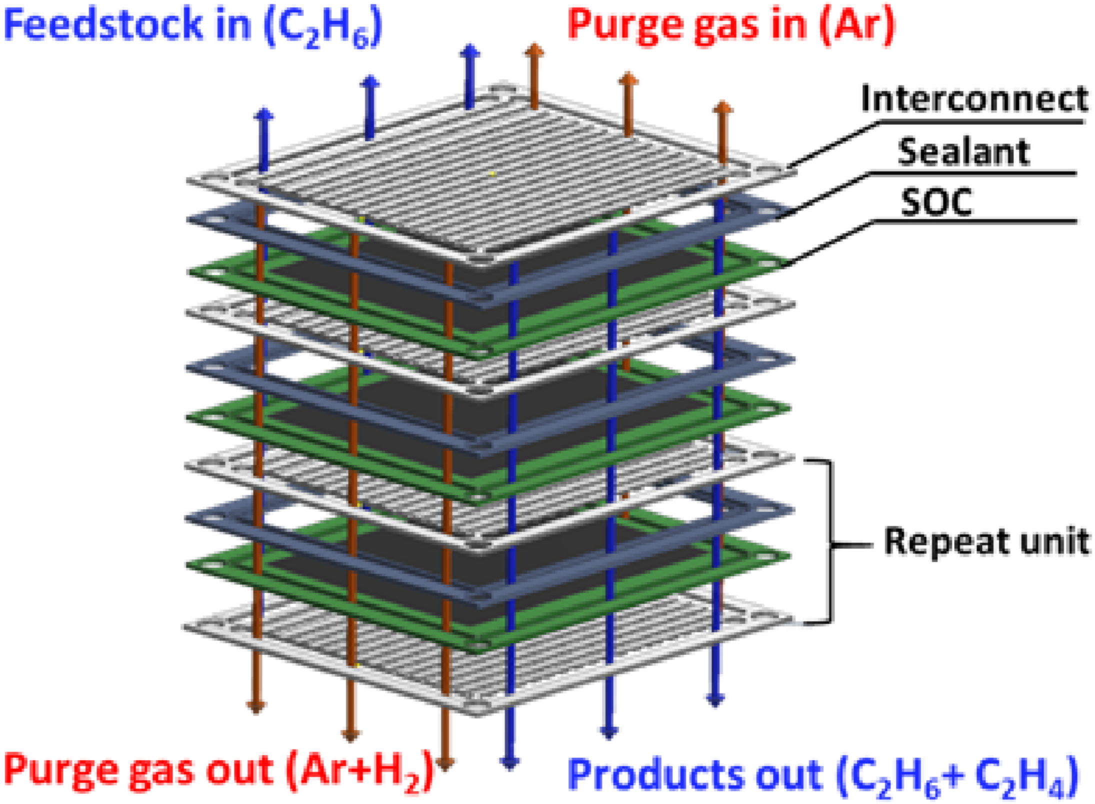

Figure C- 2. Diagram for one cell unit and cell stacks

Table C- 2. Material cost for stack cells

Items	Value	Unit
One unit:		
Interconnector	0.2	$/piece
Sealant	0.1	$/piece
Single cell (solid-oxide cell)	0.5	$/piece
Cost of one unit material:	0.8	$/piece
Height of one unit	3	mm
Number of unit of one stack	300	
Height of one stack	900	mm

Material cost of one stack:	240	$/stack
Fabrication cost:		
Total cost of one stack		

Table C- 3. Material cost for one module.

Items	**Value**	**Unit**
One module:		
Number of stacks	40	
Diameter of Container	1.5	m
Cost of stacks	9600	$
Cost of tray for stacks	1000	$
Cost of container	2000	$/piece
Material cost of one stack:	12,600	$/module

Appendix D

Compressor System Design

Appendix D

Compressor System Design

For gas compression after the ENDP product stream has been cooled via the exchanger, a turbine driven centrifugal compressor is utilized to perform compression, and there are typically multiple stages, with intermediate cooling. The number of stages necessary depends primarily upon gas composition and temperature level of the cooling medium. All the throughput of the ethylene plant will pass through gas compressors, so performance and reliability of this unit are especially important. The compressor is also an extremely expensive piece of equipment, resulting in a large percentage of the overall capital of the plant.

Appendix E

Heat Exchanger Design

Appendix E

Heat Exchanger Design

HEX1

Exchange specification: hot outlet/cold inlet temperature difference at 10°C. Its design specifications and temperature-duty curve are shown in Table E- 1 and Figure E- 1.

Table E- 1. Design specifications for HEX1

Calculated heat duty	321.186591	MMBtu/hr
Required exchanger area	87386.3486	sqft
Actual exchanger area	87386.3486	sqft
Percent over (under) design		
Average U (Dirty)	149.693656	Btu/hr-sqft-R
Average U (Clean)		
UA	13081182	Btu/hr-R
LMTD (Corrected)	13.6407394	C
LMTD correction factor	1	
Thermal effectiveness		
Number of transfer units		
Number of shells in series	1	
Number of shells in parallel		

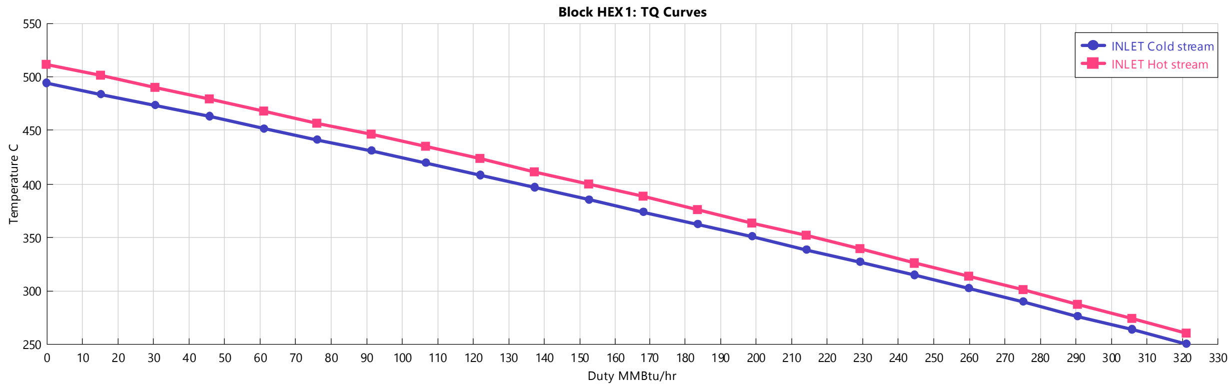

Figure E- 1. Temperature-duty curve for the HEX1.

HEX3

Exchange specification: cold outlet temperature at 30°C. This because the stream enters the membrane separtion system which requires normal temperature. See Table E- 2 and Figure E- 2.

Table E- 2. Design specificationsfor HEX3.

Calculated heat duty	9.424065	MMBtu/hr
Required exchanger area	67.13237	sqft
Actual exchanger area	67.13237	sqft
Percent over (under) design	0	
Average U (Dirty)	149.6937	Btu/hr-sqft-R
Average U (Clean)		
UA	10049.29	Btu/hr-R
LMTD (Corrected)	520.9912	C
LMTD correction factor	1	
Thermal effectiveness		
Number of transfer units		
Number of shells in series	1	
Number of shells in parallel		

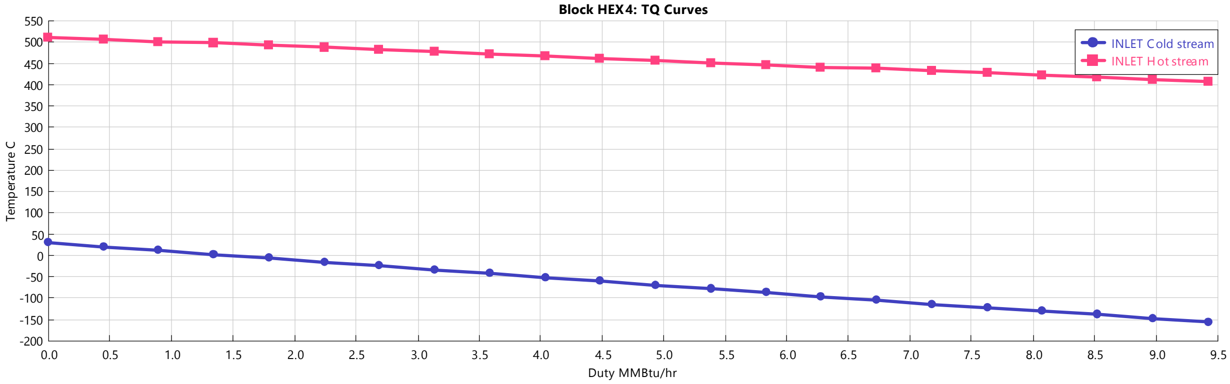

Figure E- 2. TQ curve for HEX3

Appendix F

Distillation Column Separation Design

Appendix F

Distillation Column Separation Design

All distillation columns are designed in two steps. First, columns are simulated using the DSTWU method in AspenPlus in order to obtain preliminary data, including minimum reflux ratio, minimum number of stages, and feed stage. Then RadFrac method is applied to simulate the columns for detailed design information.

The fractionation section receives the compressed ethylene-product streams at a pressure of 150 psi for further fractionation into different products and fractions at specified qualities. This is done through a series of distillation columns. Cryogenic separation is the predominant method for industrial cracked-gas separation. Membrane technology has also made significant progress in the recent past, especially on hydrogen and methane separation, which has demonstrated in commercial applications. In addition, membrane separation for ethane and ethylene is under developing and has promising results under pilot-scale studies. Therefore, separation for hydrogen and nitrogen from methane, hydrogen from nitrogen, and ethylene from ethane are model using membrane separation, while other hydrocarbon separation is conducted using distillation columns.

At current industrial practice, three processing routes have gained commercial importance, with the main characteristics being the first separation step. These routes are demethanizer, deethanizer, and depropanizer (Emerson 2010). The following is a listing of the various distillation columns and their functions:

Demethanizer. Demethanization of the produced gas separates methane as an overhead component from C_2 and heavier bottom components. Concurrently, hydrogen is removed from the produced-gas stream and may be obtained as a product by purification before or after demethanization. Methane is typically used as a plant fuel or sold. C_2 and heavier components are sent to the recovery system.

Deethanizer. Deethanization of produced gas separates acetylene, ethylene, and ethane as overhead components from C_{3+} bottom components.

Depropanizer. Depropanization separates propane and lighter fractions as overhead components from C_{4+} fractions as bottom components.

C_2 splitter or ethylene fractionation. Ethylene fractionation separates ethylene as a high-purity overhead product from ethane, which is recycled for the ENDP reactor.

C_3 splitter or propylene fractionation. Propylene fractionation separates propylene as a chemical grade overhead product or more frequently as polymer-grade propylene from propane. Propane is sold as co-products.

1. Demathanizer column for separation of CH_4, H_2, and N_2 from other HCs (**CH4H2SEP**)

   This column is a demethanizer in order to evaporate methane, hydrogen and nitrogen from other hydrocarbons (HCs). Its design is: 10 trays, feed at tray 3, and RR=0.5. It is worth noting that the top condenser is counted as the number one tray, and the bottom reboiler is as the last tray. Its performance characteristics are obtained from AspenPlus simulation and is listed as in the following tables.

Table F- 1. Separation efficiency of the demethanizer column.

Component	Overhead Light recovery	Bottom Heavy recovery
Ethane	2.10E-06	1
Ethylene	9.78E-05	0.999902171
Hydrogen	1	1.36E-13
Nitrogen	1	4.36E-09
Methane	0.99920964	0.000790364
1-But-01	1.57E-14	1
Propane	1.44E-10	1
Propy-01	1.14E-09	1

Table F- 2. Column condenser performances.

Name	Value	Units
Temperature	-155.038	C
Subcooled temperature		
Heat duty	-7.46384	MMBtu/hr
Subcooled duty		
Distillate rate	3758.155	lbmol/hr
Reflux rate	1879.077	lbmol/hr
Reflux ratio	0.5	

Table F- 3. Column reboiler performances.

Name	Value	Units
Temperature	-34.573	C
Heat duty	123.3502	MMBtu/hr
Bottoms rate	29945.07	lbmol/hr
Boilup rate	23932.66	lbmol/hr
Boilup ratio	0.799219	

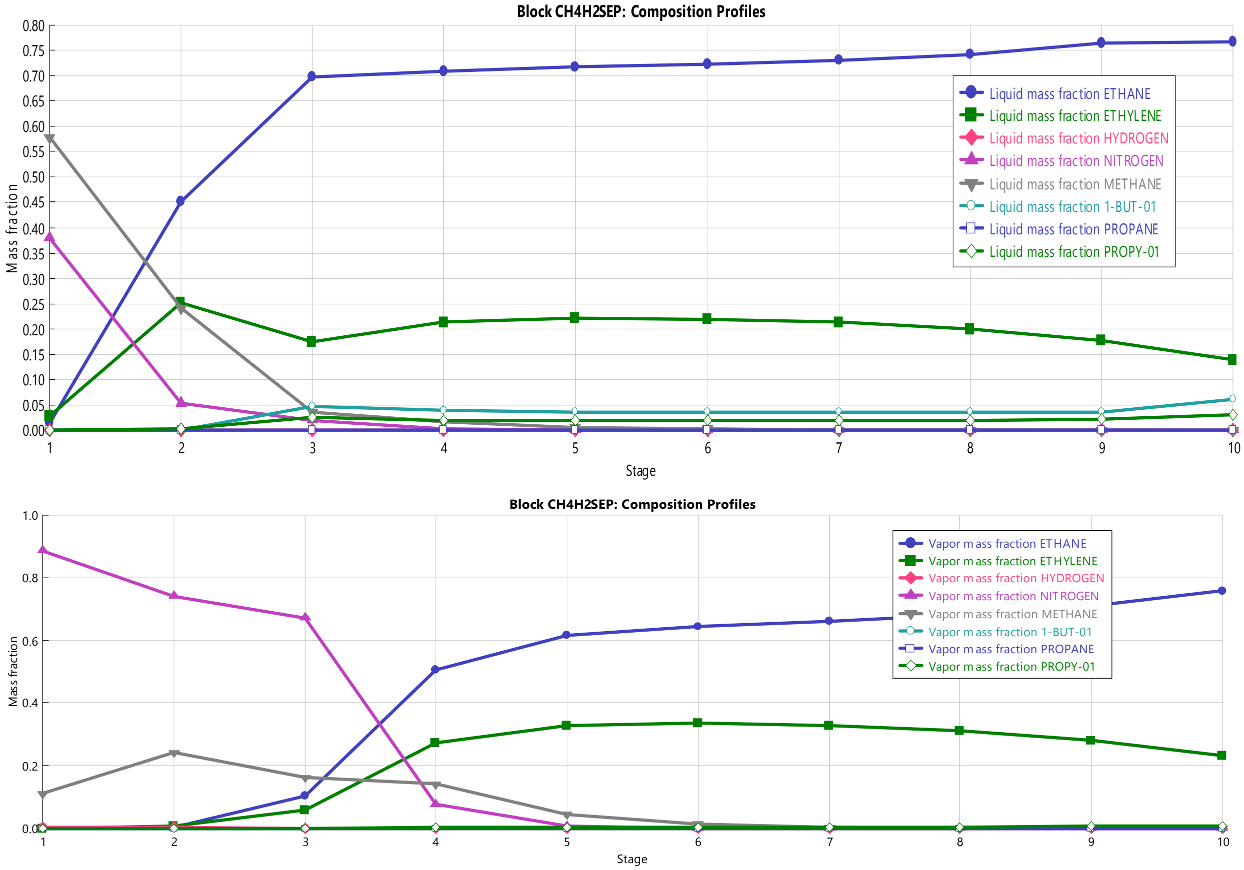

Figure F- 1. Composition profile for the column CH4H2SEP

2. Deethylenizer column for separation of C_2H_4 and C_2H_6 from other heavy HCs (**C2SEPLT**)

   This column is a de-ethanizer in order to distillate ethane and ethylene from other heavy hydrogrocarbons. Its design comprises 15 trays, with feed at Tray 7, and RR = 0.7. Its performance characteristics are obtained from AspenPlus simulation and are listed in Table F- 4, Table F- 5, and Table F- 6.

Table F- 4. Separation efficiency of the demethanizer column.

Component	Overhead Light recovery	Bottom Heavy recovery
Ethane	0.99969944	0.00030056
Ethylene	0.99999462	5.38E-06
Nitrogen	1	0.00E+00
Methane	1	1.16E-11
1-But-01	7.73E-08	1
Propane	0.00112236	0.998877644
Propy-01	0.00971688	0.990283125

Table F- 5. Column condenser performances.

Name	Value	Units
Temperature	-38.3219	C
Subcooled temperature		
Heat duty	-103.072	MMBtu/hr
Subcooled duty		
Distillate rate	2.83E+04	lbmol/hr
Reflux rate	19784.71	lbmol/hr
Reflux ratio	0.7	

Table F- 6. Column reboiler performances.

Name	Value	Units
Temperature	43.86794	C
Heat duty	251.1963	MMBtu/hr
Bottoms rate	1733.75	lbmol/hr
Boilup rate	34513.45	lbmol/hr
Boilup ratio	19.90683	

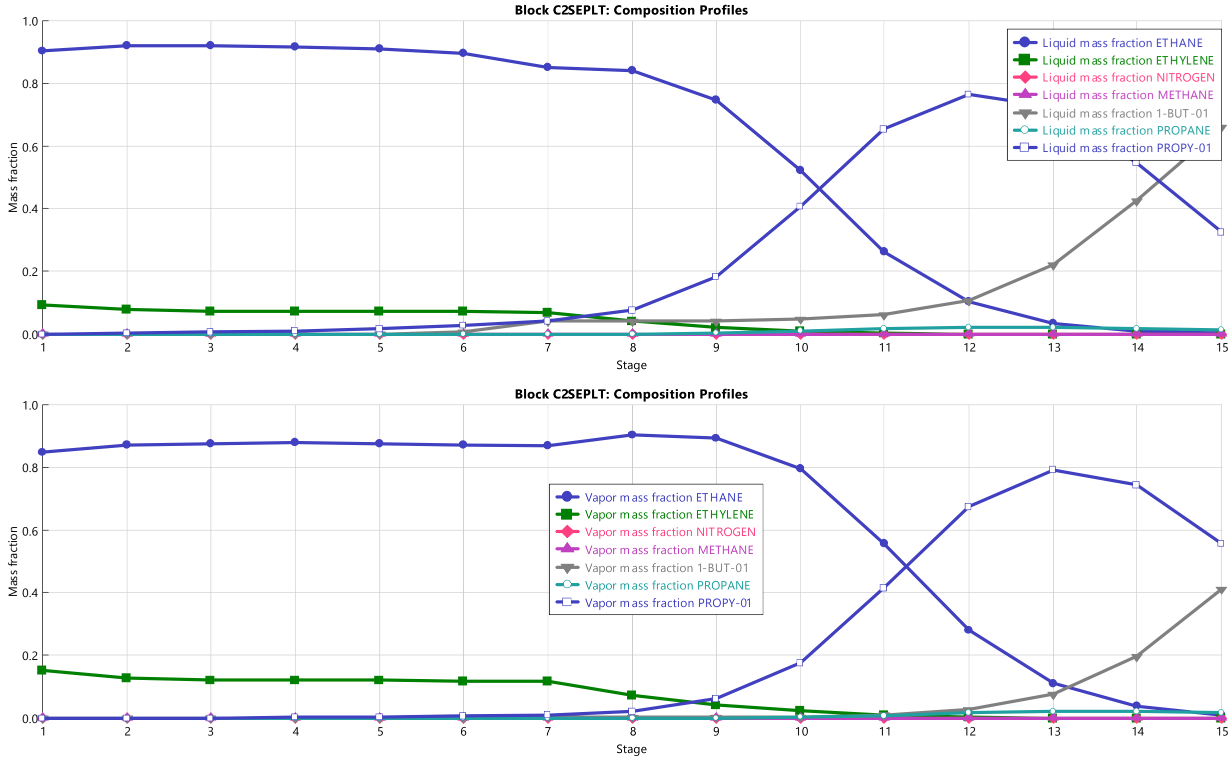

Figure F- 2. Composition profile for the column C2SEPLT

3. Depropanizer column for separation of C3 from C4 HCs (**C3C4SPLT**)

   This column is a de-propanizer in order to separate C3 HCs from C4 HCs. Its design is: 15 trays, feed at tray 8, and RR=3. Its performance characteristics are obtained from AspenPlus simulation and is listed in Table F- 7, Table F- 8, and Table F- 9.

Table F- 7. Separation efficiency of the demethanizer column.

Component	**Overhead Light recovery**	**Bottom Heavy recovery**
Ethane	0.99998923	1.08E-05
Ethylene	1	1.02E-06
Methane		
1-But-01	0.00649265	0.993507351
Propane	0.97490456	0.025095444
Propy-01	0.9910262	0.008973804

Table F- 8. Column condenser performances.

Name	**Value**	**Units**
Temperature	16.0507	C
Subcooled temperature		
Heat duty	-13.9785	MMBtu/hr
Subcooled duty		
Distillate rate	706.296	lbmol/hr
Reflux rate	2118.888	lbmol/hr
Reflux ratio	3	

Table F- 9. Column reboiler performances.

Name	**Value**	**Units**
Temperature	69.618	C
Heat duty	23.05013	MMBtu/hr
Bottoms rate	1027.454	lbmol/hr
Boilup rate	3096.82	lbmol/hr
Boilup ratio	3.014073	

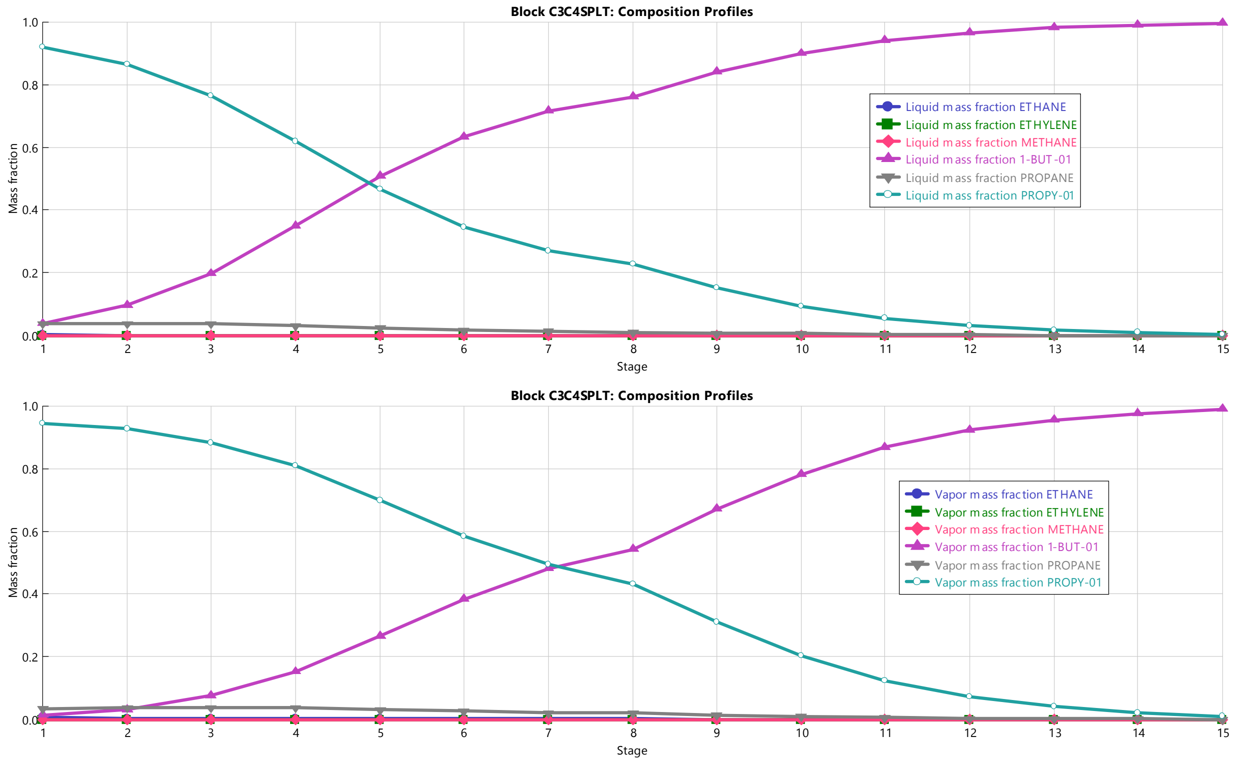

Figure F- 3. Composition profile for the column C3C4SPLT

4. C_3 splitter column for separation of C_3H_6 and C_3H_8 (**C3SEPLT**)

   This column is a C_3 splitter in order to split propylene at the overhead from propane at the bottom. Its design is: 40 trays, feed at tray 20, and RR=6. Its performance characteristics are obtained from AspenPlus simulation and is listed as in the following tables.

Table F- 10. Separation efficiency of the demethanizer column.

Component	**Overhead Light recovery**	**Bottom Heavy recovery**
Ethane	1	1.77E-12
Ethylene	1	1.52E-15
Methane		
1-But-01	5.61E-10	1
Propane	0.52836926	0.471630737
Propy-01	0.95034708	0.049652921

Table F- 11. Column condenser performances.

Name	**Value**	**Units**
Temperature	11.32666	C
Subcooled temperature		

Heat duty	-30.1644	MMBtu/hr
Subcooled duty		
Distillate rate	655.1166	lbmol/hr
Reflux rate	3930.699	lbmol/hr
Reflux ratio	6	

Table F- 12. Column reboiler performances.

Name	Value	Units
Temperature	20.89526	C
Heat duty	30.51866	MMBtu/hr
Bottoms rate	51.17938	lbmol/hr
Boilup rate	4627.47	lbmol/hr
Boilup ratio	90.41667	

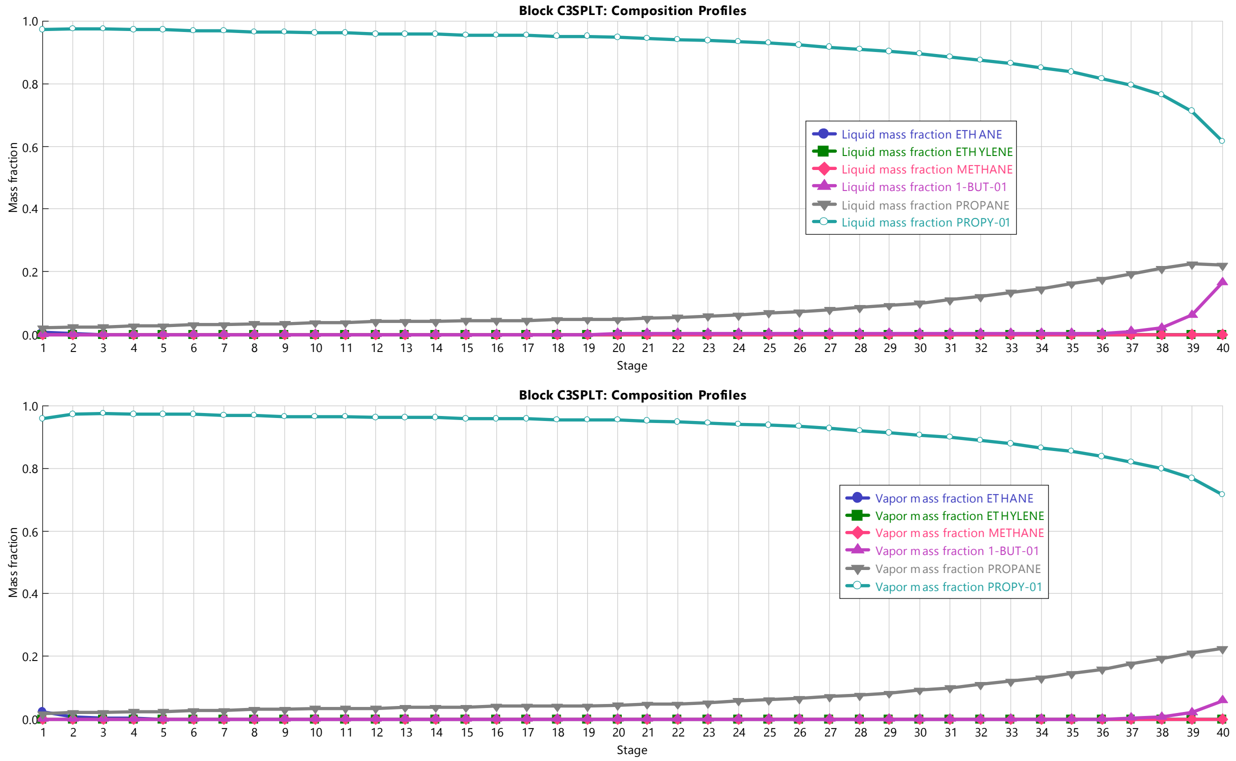

Figure F- 4. Composition profile for the column C3SPLT.

C_2 splitter column for separation of C_2H_6 and C_2H_4 (C2SPLT)

This column is a C_2 splitter in order to split ethylene at the overhead from ethane at the bottom. Its design is: 40 trays, feed at tray 20, and RR=10. Its performance characteristics are obtained from AspenPlus simulation and is listed as in the following tables

Table F- 13. Separation efficiency of the demethanizer column

Component	Overhead	Bottoms
Ethane	0.000252	0.999748
Ethylene	0.989377	0.010623
Nitrogen	1	0
Methane	1	0
1-BUT-01	0	1
Propane	0	1
Propy-01	0	1

Table F- 14. Column condenser performances.

Name	Value
Temperature (°C)	-59.7883
Subcooled temperature	
Heat duty (MMBTU/hr)	-280.622
Subcooled duty	
Distillate rate (lbmol/hr)	5706.511
Reflux rate (lbmol/hr)	57065.11
Reflux ratio	10
Free water distillate rate	
Free water reflux ratio	
Distillate to feed ratio	0.989969

Table F- 15. Column reboiler performances.

Name	Value
Temperature (°C)	-35.7491
Heat duty (MMBTU/hr)	212.3583
Bottoms rate (lbmol/hr)	13062.02
Boilup rate (lbmol/hr)	40661.76
Boilup ratio	3.112977
Bottoms to feed ratio	2.266007

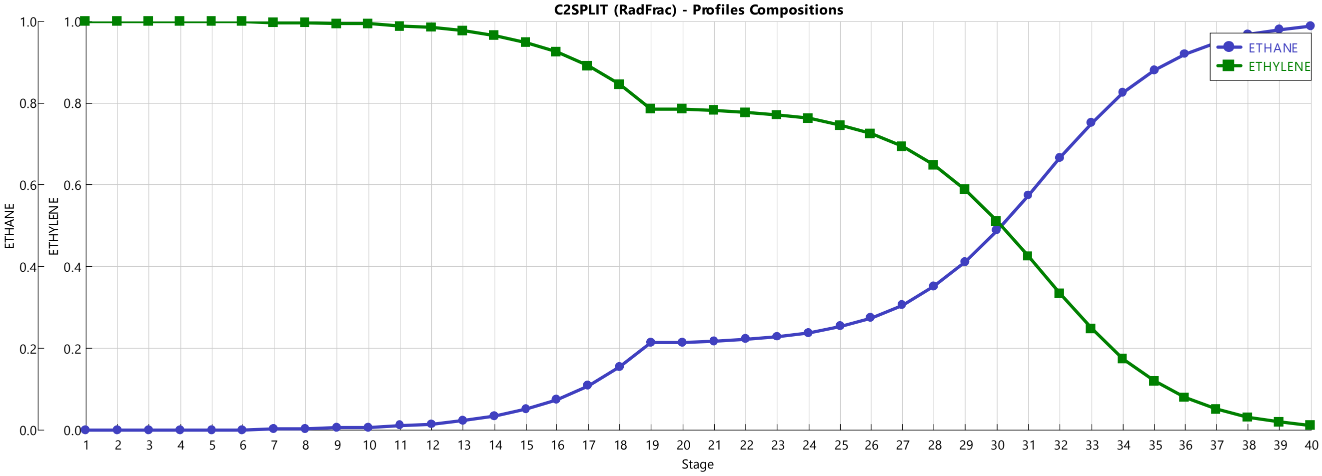

Figure F- 5. Composition profile for the column C2SPLT.

Appendix G

Membrane Separation Design

Appendix G

Membrane Separation Design

Membrane Gas Separations (CAPEX and OPEX) –

Details of the hydrogen and ethylene separations are given within this section.

Hydrogen Separations

Honeywell UOP, LLC (Polysep), and Air Products & Chemicals, Inc. (PRISM), will have proprietary hydrogen separations that can accomplish these capacities. Both membrane separation systems will have similar CAPEX, and potentially, they could have similar OPEX. A major problem with this separation is the pressure needed for these systems; thus, the costs can change. This is for a 90–99% recovery of hydrogen gas. Air Products recommends that the pressures to be increased 1000 from 130 psi. The estimate from Air Products gives a good indication of the expenses involved in these systems. In addition, the expenses can have a larger variance (up to 20%) to the CAPEX and OPEX than shown due to gas contaminates and swelling gases. Also, *in-house* cost estimates on these calculations are provided by INL.

Response from Air Products' evaluation at 130 psi,

> *Due to the low pressure and low-pressure ratio, these targets are not mutually achievable. Based on an initial screening evaluation (1000 psi), the maximum achievable H_2 purity would be approximately 93%, at 94% H_2 recovery. The achievable purity increases to approximately 95% when the H_2 recovery is dropped to 90%. The indicative price of the first system (93% purity / 94% recovery) is US$ 3,500,000.00.*

- *For both membrane systems,* the estimated CAPEX for the hydrogen recovery systems (90–99%) can range from $10–15M, and the OPEX for these systems can be $3–8M/yr.
- *Not possible at 130 psi,* a huge membrane surface area is needed for this separation; therefore, the CAPEX will be high and requires a large footprint for this membrane setup.
    - Estimated CAPEX: $11.5M
    - Estimated OPEX: $2.7M/yr
- *At 1000 psi (recommended by Air Products),* the membrane surface area is within reason, but pumps are required to achieve the pressure. This will reduce the size of the separations unit and provide optimal separations for their membranes.
    - Estimated CAPEX: $2.9M
    - Estimated OPEX: $8.8 M/yr
    - ***Air Products' evaluation on CAPEX: $3.5M, No OPEX was given.***

Ethylene/Ethane (C_2) Separation

Imtex (Permylene) and Compact Membrane Systems (Optiperm) could have capacity for this C_2 separation. This is for a 90–99% recovery of ethylene. One issue with either system is that each was tested at a pilot-plant scale, and not at the capacities requested (Imtex was tested at nearly 100 times less capacity). Because these industrial membranes are not explicitly explained for their permeance and ethylene separations, their calculations at a pilot-plant scale are used. Thus, the cost of these systems might have a larger variance (up to 20%) to the CAPEX and OPEX than shown.

- For Imtex membrane system:

  - Estimated CAPEX: $50–150M
  - Estimated OPEX: $30–60M/yr.
- For Compact Membrane Systems membrane system:
  - Estimated CAPEX: $70–150M
  - Estimated OPEX: $15–40M.

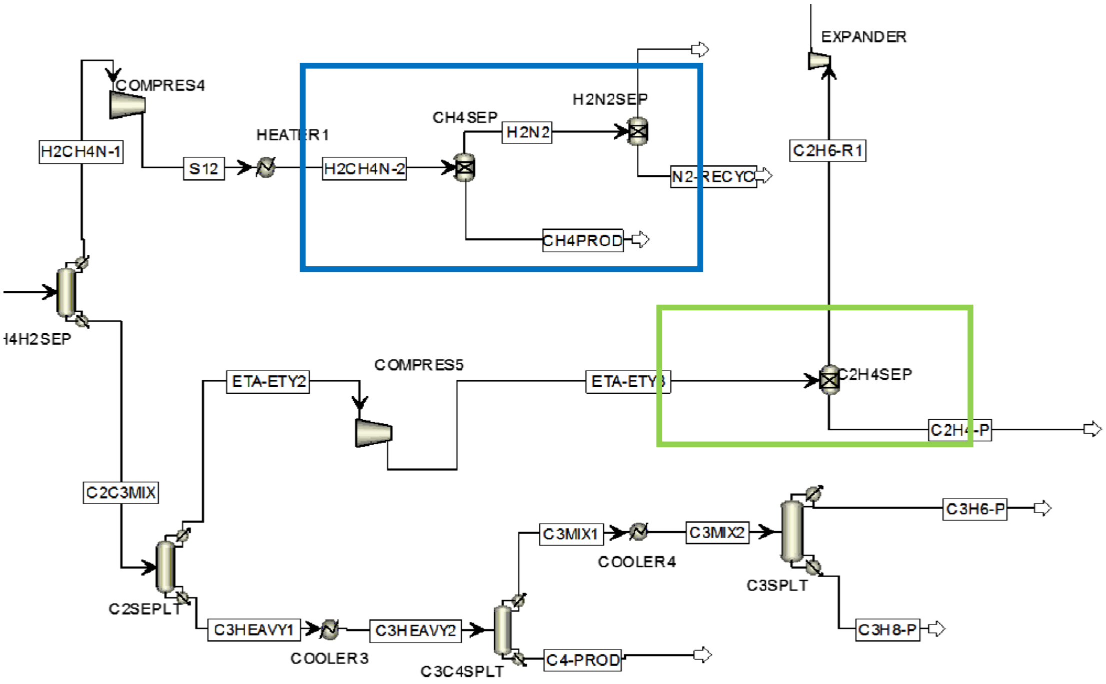

Figure G - 1. Hydrogen separations (blue) and ethylene separations (green).

Table G - 1. Mass flow rate of streams for membrane process design

	H_2CH_4N-2	**H_2N_2**	**H_2-P_2**	**N_2-Recyc**	**ETA-ETY3**	**C_2H_4-P**	**C_2H_6-R1**
Vol. Flow (ft^3/hr)	20780.15	218428.6	16091.82	202279.4	151504	41510.25	123838.8
Ethane	0	0	0	0	126,952	2,104	123,081
Oxygen	0	0	0	0	0	0	0
Ethylene	3	0	0	0	24,514	39,406	720
Hydrogen	1,212	14,720	14,046	736	0	0	0
Nitrogen	16,092	203,665	2,046	201,499	0	0	0
Methane	3,474	44	0	44	3	0	3
1-But-01	0	0	0	0	0	0	0
Propane	0	0	0	0	0	0	0
Propy-01	0	0	0	0	35	0	35
Carbon	0	0	0	0	0	0	0
Water	0	0	0	0	0	0	0

CO_2	0	0	0	0	0	0	0

Membrane Separations

Hydrogen Volume Flows

Volume Flow, total H_2CH_4-2 - 19252 ft^3/hr [membrane in]; 130 psi

Volume Flow, total H_2-2 - 25407 ft^3/hr [membrane out]; 80 psi

Volume Flow, total CH_4-PROD - 3617 ft^3/hr [membrane out]; 130 psi

Mole Flow, total H_2CH_4-2 - 427 lbmol/hr [787 kg/hr]; 130 psi

Mole Flow, total H_2-2 - 347 lbmol/hr [318 kg/hr]; 80 psi

Mole Flow, total CH_4-PROD - 80 lbmol /hr [469 kg/hr]; 130 psi

Temperature, 30°C (ambient); 303 K

Hydrogen Separations (Blue box in Figure G-1)

A factor that should be noted is the pressure differential among these membrane systems. Because the pressure is relatively small for this application, the overall hydrogen separations can be diminished using polymer membranes. Most polymer membrane systems for hydrogen are designed to operate at multiple bars (>10 bars; ~150 psi), and the current pressures are at 130 psi. For example, industrial membrane systems utilize pressures at 1000–1200 psi, and this will decrease the size of the separation unit, but add cost to pressurize the system. Air Products recommends that the pressure to be increased to 1000 psi for optimal operations—not that the requested pressures will change the separations. However, lower pressures will increase the square area needed for the separations unit and increase capital cost. Nonetheless, these industrial membrane-module designs should accommodate the capacity for these larger flows at the requested pressures. These membrane modules are hollow fibers or spiral wound, which can be custom designed with surface areas between 1–200 m^2. Also, the calculated hydrogen gas will have a purity range between 90–99%.

Both UOP and Air Products membrane modules can be effective at this separation due to pressure requirement and temperatures that are closer to those requested. The capacity for both membrane systems should be possible with these large gas flows.[1] The blue box in Table G - 2 highlights the gas selectivity of H_2/CH_4, and the red boxes are for the polymers for UOP (cellulose acetate), Air Products (polysulfone), and UBE Industries, LTD (polyimide-BPDA).

As a side note, UBE has a polymer membrane that has better selectivity and permeability (at 60°C), but it must be custom made for this separation system that will add more cost than the others. In addition, UBE membrane manufacturing plants are in Japan.

- UOP (USA): selectivity for H_2/CH_4 is 67 and a permeability of 24 Barrers (at 25°C).
- Air Products (USA): selectivity for H_2/CH_4 is 56 and a permeability of 14 Barrers (at 35°C).
- UBE (Japan) - selectivity for H_2/CH_4 is 125 and a permeability of 50 Barrers (at 60°C).
- 1 Barrer = 10^{-10} [(cm^3 cm)/(cm^2 s cmHg)]
- 1 Barrer = 3.35×10^{-16} [(mol m)/(m^2 s Pa)]

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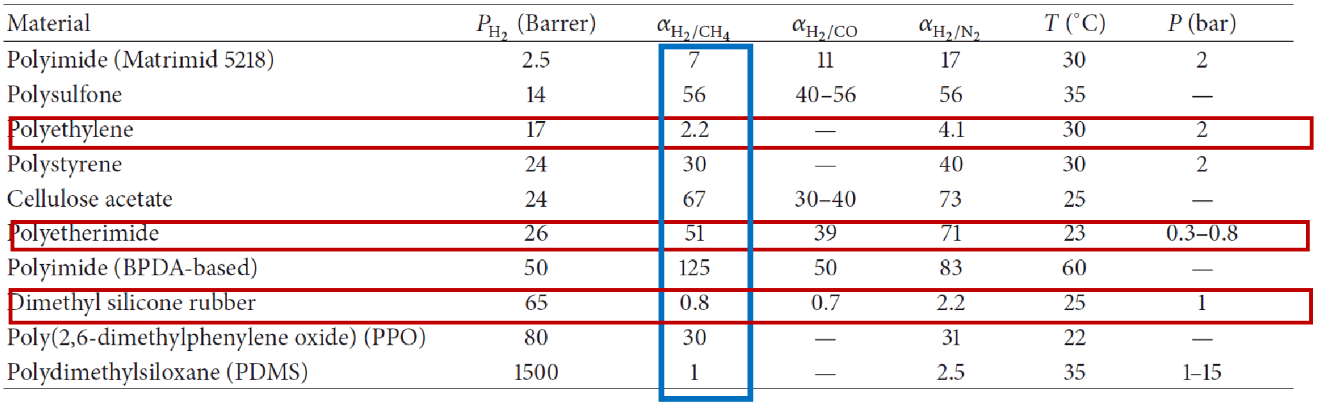
[1] Y. Alqaheem, A. Alomair, M. Vinoba, and A. Pérez, “Polymeric Gas-Separation Membranes for Petroleum Refining,” https://www.hindawi.com/journals/ijps/2017/4250927/. https://doi.org/10.1155/2017/4250927.

Table G - 2. Hydrogen permeability and selectivity of different membrane materials. [Source]



Material	P_{H_2} (Barrer)	α_{H_2/CH_4}	$\alpha_{H_2/CO}$	α_{H_2/N_2}	T (°C)	P (bar)
Polyimide (Matrimid 5218)	2.5	7	11	17	30	2
Polysulfone	14	56	40–56	56	35	—
Polyethylene	17	2.2	—	4.1	30	2
Polystyrene	24	30	—	40	30	2
Cellulose acetate	24	67	30–40	73	25	—
Polyetherimide	26	51	39	71	23	0.3–0.8
Polyimide (BPDA-based)	50	125	50	83	60	—
Dimethyl silicone rubber	65	0.8	0.7	2.2	25	1
Poly(2,6-dimethylphenylene oxide) (PPO)	80	30	—	31	22	—
Polydimethylsiloxane (PDMS)	1500	1	—	2.5	35	1–15

UOP LLC, Honeywell Company, Polysep (Cellulose Acetate)

UOP Polysep is a membrane for hydrogen production that can treat refinery off-gases. The membrane operates at temperatures of 60–82°C, with feed pressures of 14–170 bar. PolySep can handle a larger volume (412,010 m^3/hr). The permeate pressure ranges from 4–84 bar with hydrogen recovery of 70–98%.

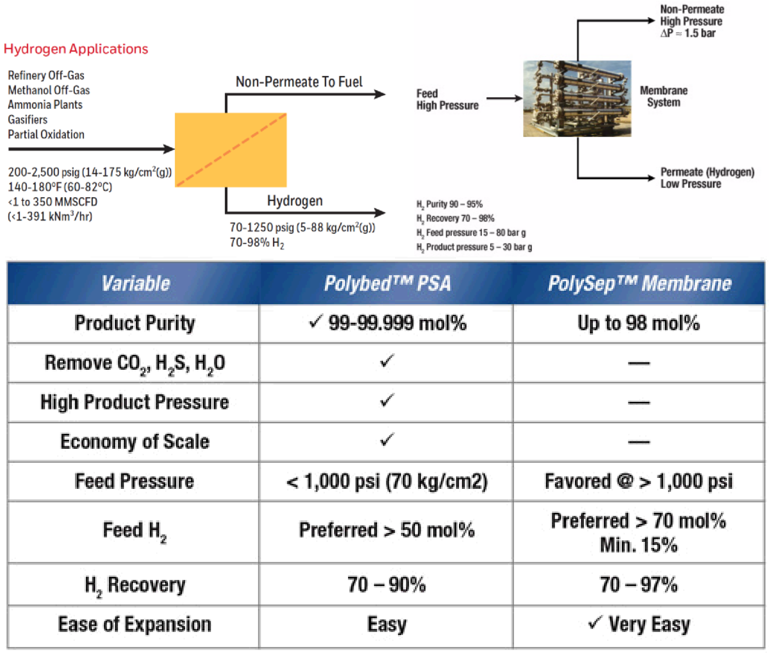
From UOP's Brochure on Hydrogen Separations:

The UOP's description on hydrogen separation can be founded in the following two links. The economic justification for a PSA unit will depend on the H_2 content of the feed stream and how the customer values chemical hydrogen versus hydrogen as fuel. Generally, the following rules apply:

- Hydrogen feed concentrations >55% are easily economically justified
- Between 40 and 50% H_2 can be economically upgraded dependent on site-specific requirements
- Below 40% H_2, economics become more difficult to justify.

https://www.uop.com/?document=polysep-membrane-for-gas-extraction-purification&download=1

https://www.uop.com/processing-solutions/refining/hydrogen-management/#purify-recover



Variable	*Polybed™ PSA*	*PolySep™ Membrane*
Product Purity	✓ 99-99.999 mol%	Up to 98 mol%
Remove CO_2, H_2S, H_2O	✓	—
High Product Pressure	✓	—
Economy of Scale	✓	—
Feed Pressure	< 1,000 psi (70 kg/cm2)	Favored @ > 1,000 psi
Feed H_2	Preferred > 50 mol%	Preferred > 70 mol% Min. 15%
H_2 Recovery	70 – 90%	70 – 97%
Ease of Expansion	Easy	✓ Very Easy

Figure G - 2. UOP hydrogen separation process.

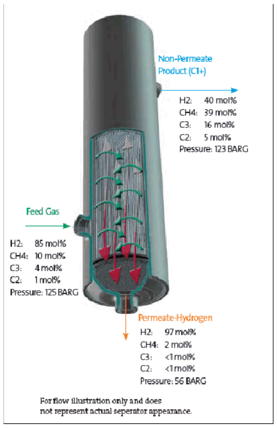
Air Products, PRISM (Polysulfone)

PRISM modules are made for nitrogen purification; however, they can be used for hydrogen separations from refinery and petroleum separations (see below). The maker claims that its membranes are fully capable of enriching hydrogen from organic feed streams, where packaged PRISM hydrogen generators are designed to meet requirements up to 5,000 normal m^3/hr (176573 ft^3/hr; 4.56 million ft^3/day).

From Air Products' brochure on hydrogen separations:

http://www.airproducts.com/~/media/Files/PDF/products/supply-options/prism-membrane/en-prism-process-gas-brochure.pdf?la=en

http://www.h2alliance.com/pdf/338-12-030-GLB_CreatingValue.pdf



Features	**Adsorption**	**Membranes**	**Cryogenics**
H_2 Purity	99.9%+	90 – 98%	90 – 96%
H_2 Recovery	75 – 92%	85 – 95%	90 – 98%
Feed Pressure	10 – 40 barg	20 – 160 barg	> 5 – 75 barg
Feed H_2 Content	> 40%	>25 – 50%	> 10%
H_2 Product Pressure	Feed Pressure	<< Feed Pressure	Feed / Low Pressure
H_2 Capacity	1 – 225 K Nm^3 /hr	1 – 50+ K Nm^3 /hr	10 – 75+ K Nm^3 /hr
Pretreatment Requirements	None	Minimum	CO_2, H_2O Removal
Multiple Products	No	No	Liquid HC's
Capital Cost	Medium	Low	Higher
Scale Economics	Moderate	Modular	Good

Figure G - 3. Specifications on Air Products, Prism^{TM}.

Estimated Calculation of Polymer Surface Area

Hydrogen density: 0.08988g/L = 8.988×10^{-5} g/cm3

Methane density: 5.54×10^{-4} g/cm3

787 kg/hr *total* (85.5% is hydrogen, 14.4% is methane) = 218.6 g/s *total*

Covert g to cm3 of gas flow (per second)

Hydrogen is $(0.855 \times 218.6 \text{ g/s}) / 8.988 \times 10^{-5} \text{ g/cm3} = 2079473 \text{ cm}^3\text{/s}$

Methane is $(0.144 \times 218.6 \text{ g/s}) / 5.54 \times 10^{-4} \text{ g/cm3} = 56820 \text{ cm}^3\text{/s}$

Estimated membrane thickness is 0.0001 cm or 1 micron.

Pressure at 130 psi or 672.3 cmHg

1 Barrer = $[(\text{cm3 cm})/(\text{cm2 s cmHg})]\ 10^{-10}$

Permeability for polysulfone (PRISM) is 14 Barrers

$14 \text{ cm}^3 \text{ cm/cm}^2 \text{ s cmHg} = [((2079473 \text{ cm}^3\text{/s} + 56820 \text{ cm}^3\text{/s}) \times 0.0001 \text{ cm})/ (672.3 \text{ cmHg})] / (10^{-10})$

$14 /\text{cm}^2 = [(2136293 \times 0.0001)/672.3] / (10^{-10})$

$14 /\text{cm}^2 = 0.340554 /(10^{-10})$

$\text{cm}^2 = 243252857$

Surface area for this separation is **24325 m2** for a 1-micron film thickness

Permeability for cellulose acetate (Polysep) is 24 Barrers

24 cm^3 cm/cm^2 s cmHg = [(2079473 cm^3/s + 56820 cm^3/s) X 0.0001 cm)/ (672.3 cmHg)] / (10^{-10})

24 /cm^2 = [(2136293 × 0.0001)/672.3] / (10^{-10})

24 /cm^2 = 0.340554 / (10^{-10})

cm^2 = 141897500

Surface area for this separation is **14190 m^2** for a 1-micron film thickness

Pressure at 1000 psi or 5171.5 cmHg (recommended by Air Products)

1 Barrer = [(cm3 cm)/(cm2 s cmHg)] 10^{-10}

Permeability for polysulfone (PRISM) is 14 Barrers

14 cm^3 cm/cm^2 s cmHg = [((2079473 cm^3/s + 56820 cm^3/s) × 0.0001 cm)/ (5171.5 cmHg)] / (10^{-10})

14 /cm^2 = [(2136293 × 0.0001)/ 5171.5] / (10^{-10})

14 /cm^2 = 0.041309 /(10^{-10})

cm^2 = 29506428

Surface area for this separation is **2951 m^2** for a 1-micron film thickness

Permeability for cellulose acetate (Polysep) is 24 Barrers

24 cm^3 cm/cm^2 s cmHg = [(2079473 cm^3/s + 56820 cm^3/s) × 0.0001 cm)/ (5171.5 cmHg)] / (10^{-10})

24 /cm^2 = [(2136293 × 0.0001)/ 5171.5] / (10^{-10})

24 /cm^2 = 0.041309 / (10^{-10})

cm^2 = 14189750

Surface area for this separation is 1721 m^2 for a 1-micron film thickness

The rationale for showing these different sets of calculations is to reveal the difference in membrane surface area using different pressures. Also, it estimates the square area that the membrane separation unit (system) will occupy at the refinery. At 130 psi, the calculated module design will be roughly 20000–30000 m^2 surface area; however, the actual membrane surface area could be larger due to the low driving force. At 1,000 psi, the membrane surface areas drop to 2000–3000 m^2. Air Products gave a cost estimate for the CAPEX and OPEX of these modular units, and it can be assumed that the UOP will be similar in capital costs and operational costs.

Costs for Hydrogen Separations

Air Products provided the initial information to the CAPEX to their system, which is $3.5M.

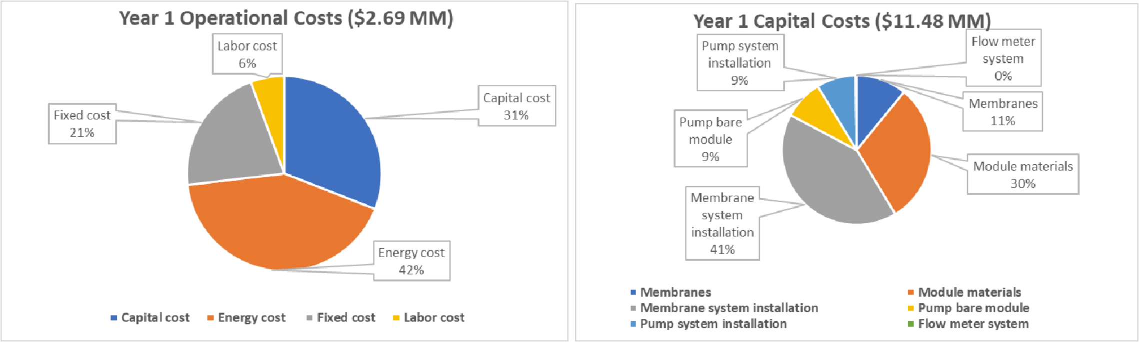
> *Based on the provided figures, it appears that your target is 94% H2 recovery at 99% H_2 Purity. However, due to the low pressure and low-pressure ratio, these targets are not mutually achievable. Based on an initial screening evaluation, the maximum achievable H_2 purity would be approximately 93%, at 94% H_2 recovery. The achievable purity increases to approximately 95% when the H2 recovery is dropped to 90%. The indicative price of the first system (93% purity / 94% recovery) is US$ 3,500,000.00.*

Note: These calculations were *in-house* (INL) cost estimates. They provide an order-of-magnitude cost estimate that is relevant to the requested hydrogen gas separation.

The technoeconomic calculations were performed for H_2-CH_4-ethylene-ethane separation system. The major capital investments for the system are pumps, membranes, membrane modules, and costs associated with the installation. The operation costs consist of payments for the capital cost (6% yearly interest on capitals), energy cost, fixed costs and labor. The basis of all calculations is 787 kg/hr feed input to the system and 8000 hr per year of operation. Fifty dollars per square meter is assumed to be the cost of the membrane for all these calculations, and \$0.12/kWh electricity cost is assumed. The materials of the module used is stainless steel.

[NOT POSSIBLE AT LOW PRESSURES] 130–150 psi Hydrogen Separation System *(INL Estimate)*

Although this is not possible, INL used a program to calculate this information. For a 150 psi system, most of the operating cost is still energy cost, but capital cost has a big impact. For Year 1, total operating cost is \$2.69 MM, and the overall capital cost is \$11.48 MM. The following plots summarize the results (Figure G-4):

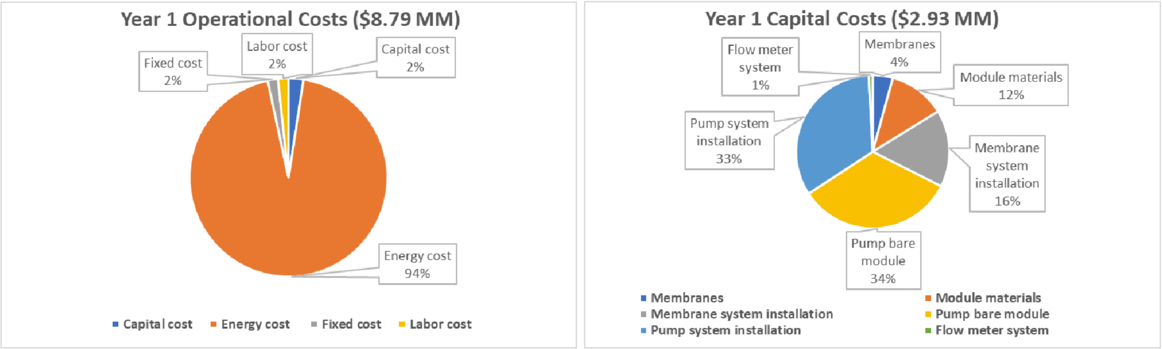


(a) (b)

Figure G - 4. (a) Year 1 OPEX summary and (b) CAPEX summary for 787 kg/hr system at 130–150 psi.

1000 psi Hydrogen Separation System *(INL Estimate)*

INL used a program to calculate this information. For 1000 psi system, most of the operating cost is for the electricity cost. For Year 1, total operating cost is \$8.74 MM, and the overall capital cost is \$2.93 MM. The following plots summarize the results (Figure G-5):



(a) (b)

Figure G - 5. (a) Year 1 OPEX Summary and (b) CAPEX Summary for 787 kg/hr system at 1000 psi.

Ethylene Separations (Green box in Figure G-1)

Ethylene Volume flows

Volume Flow, total ETA-ETY3 – 923,573 ft^3/hr [membrane in]; 130 psi

Volume Flow, total C_2H_4-P – 616,919 ft^3/hr [membrane out]; 70 psi

Volume Flow, total C_2H_6-R1 – 519,385 ft^3/hr [membrane out]; 130 psi

Mole Flow, total ETA-ETY3 – 20,503 lbmol/hr [272828 kg/hr]; 130 psi

Mole Flow, total C_2H_4-P – 7,374 lbmol /hr [93,,961 kg/hr]; 70 psi

Mole Flow, total C_2H_6-R1 – 13,129 lbmol /hr [178,867 kg/hr]; 130 psi

Temperature, 30°C (ambient); 303 K

The assumption is that membrane technologies would be used for this separation. Another assumption is that facilitated transport membranes at ambient temperatures are warranted. From these assumptions, two companies, Compact Membrane Systems (CMS) and Imtex, have shown ethylene separation modules for larger-scale separations (appropriate to pilot plants). These companies have membranes that operate close to the requested pressures and have good separations for ethylene over ethane. Their presented systems have much smaller mass-flow capacities (18123 kg/hr and 300 kg/hr) than the requested mass flows (272,828 kg/hr); therefore, this will skew these data for this separation. Presently, their membranes utilize facilitated transport mechanism, which involves silver salts for the permeation of ethylene over the other gases. These specialized membranes were recently scaled for olefin separations (C_2-C_4 alkenes), and their CAPEX and OPEX are calculated for propylene and propane (C_3) separations. The ethylene and ethane (C_2) separations should be similar in value, but the cost could be higher due to the changes in pressure needed for the C_2 separation compared to C_3 separation. These companies have provided CAPEX and OPEX for their C_3 separations, but it is assumed that these values will be closely aligned with the proposed C_2 separation. Also, the calculated ethylene gas will have a purity range between 90–99%.

Note: CMS is located in the U.S., and Imtex is in Canada. If these membrane systems need to be manufactured, the membrane systems will be assembled at the company's origin. However, both companies will have offices in the U.S. that can be contacted for further information.

Membrane Information

Compact Membrane Systems – Optiperm™ (USA) https://compactmembrane.com/wp-content/uploads/2018/10/Optiperm-white-paper.pdf Ethylene permeance 150 GPU and a selectivity of 20-80 (depending on operating conditions and feed composition)

Imtex – Permylene™ (Canada) https://www.imtexmembranes.com/hubfs/whitepapers/Imtex_Permylene-Facilitated-Transport-and-Separation-Membranes.pdf Ethylene permeance 450 scc/min (0.35-0.8 kg/m2 hr) and a selectivity of 20-80 (depending on operating conditions and feed composition)

From Compact Membrane Systems' Brochure on Olefin Separations

> *Optiperm Membrane Demonstrates Stable Performance in Pilot Study of HD5 Propane Production.* ***Production scale of the presented economic data is for 175,000 tons/yr (18123 kg/hr)***. *Compact Membrane Systems' CAPEX/OPEX estimate for the C_2 Separation is used here, and the OPEX is assumed as a yearly expense. Because the mass flow is 272828 kg/hr, the assumption is that the CAPEX/OPEX can be up to 15 times more expensive from the estimate given in Table 2. Due to the fluorinated polymer needed for their membrane, the estimation of CAPEX will be high. However, the OPEX of their membrane should be lower. This means that the estimated CAPEX is between [$70–150M] and the estimated OPEX can be estimated at [$30–60M].*

Table G - 3. Economics of commercial-scale membrane process (all costs in millions of dollars).

CAPEX, including all auxiliary equipment	13.1
OPEX, including all maintenance costs	4.9

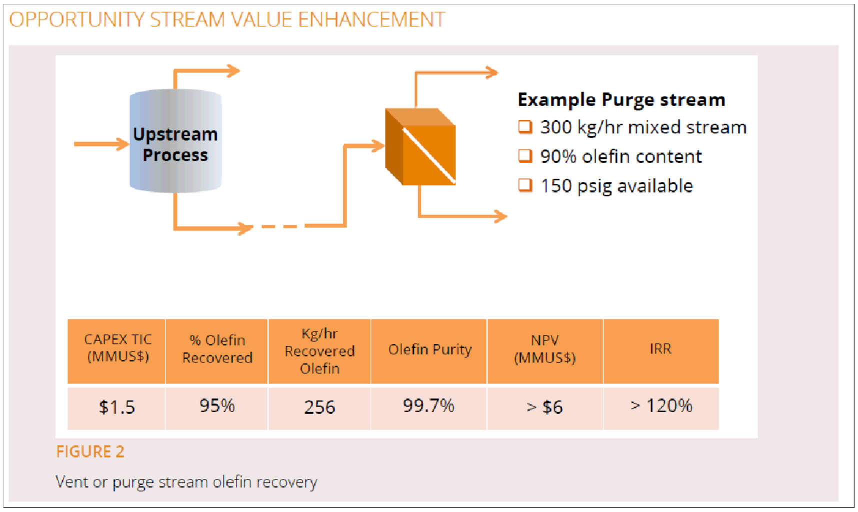
Estimated net annual benefit	10–20
Payback time	16–8

https://compactmembrane.com/wp-content/uploads/2019/10/DCRC-Pilot-Study-White-Paper.pdf

FROM IMTEX’S BROCHURE ON OLEFIN SEPARATIONS

Permylene Cost Estimate for 300 Kg/Hr (from Their White Paper)

It is expected that the cost estimates are like Optiperm™’s at the 272828 kg/hr, where the estimated CAPEX can be [$50–150M]. The OPEX will be probably close to the Optiperm™ (CMS) estimate, but maybe higher at [$30M]/yr to [60M]/yr. However, it depends on the necessary chemicals (replenish the silver salt for membrane), power (electricity), and personnel time (operation engineer/maintenance) that are needed.


OPPORTUNITY STREAM VALUE ENHANCEMENT

Example Purge stream
- ☐ 300 kg/hr mixed stream
- ☐ 90% olefin content
- ☐ 150 psig available

CAPEX TIC (MMUS$)	% Olefin Recovered	Kg/hr Recovered Olefin	Olefin Purity	NPV (MMUS$)	IRR
$1.5	95%	256	99.7%	> $6	> 120%

FIGURE 2

Vent or purge stream olefin recovery

Figure G - 6. Cost summary on IMTEX Permylene

https://cdn2.hubspot.net/hubfs/1728742/whitepapers/Whitepaper%20-%20Cost%20Effective%20Alternative%20to%20Distillation%20for%20Olefin%20Purification%20and%20Extraction.pdf?t=1498669722682

Membrane Separation

Membranes are an integral part of many industrial processes because their simple operation is often more environmentally sustainable and cost-effective than those of other separation technologies. Significant applications are in gas separations and water purification. The unit operation is simple to describe. As shown in Figure G - 7, the high-pressure feed enters the membrane unit, where molecules with higher permeability through the membrane will exit as the permeate. The retentate contains molecules that were not able to travel through the membrane.

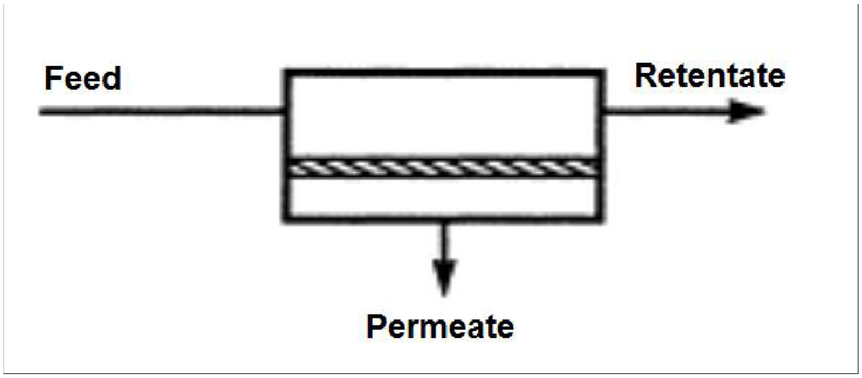


Figure G - 7. Unit operation diagram for a membrane separator.

As shown in Table G - 4, properties of five hydrogen-selective membranes are shown. Each membrane has advantages and disadvantages. Research organizations and companies continue to work to develop better versions of each.

Table G - 4. Properties of various H_2-selective membranes.

	Dense Polymer	**Microporous Ceramic**	**Dense Ceramic**	**Porous Carbon**	**Dense Metallic**
Operating Temperature (°C)	<100	200–600	600–900	500–900	300–600
H_2 Selectivity	Low	Moderate	Very High	Low	Very High
H_2 Flux	Low	High	Moderate	Moderate	High
Known Poisoning Issues	HCl, SO_X, CO_2	-	H_2S	Strong vapors, organic	H_2S, HCl, CO
Example Materials	Polymers	Silica, Al, Zr, TiO_2, zeolites	$SrCeO_3$, $BaCeO_3$	C	Palladium alloys, Pd-Cu, Pd-Au
Transport Mechanism	Solution/diffusion	Molecular sieving	Solution/diffusion	Surface diffusion, molecular sieving	Solution/diffusion

Physical Structure of Polymer Membranes

Membranes comprise two major layers: a non-porous membrane and a porous support. The non-porous membrane is where separation occurs. The purpose of the porous support is mechanical integrity, and this layer is often about 40–200 times thicker than the non-porous membrane.

Appendix H

Refrigeration System Design

Appendix H

Refrigeration System Design

The refrigeration system will further reduce the temperature of feeding stream for downstream cryogenic separation of various hydrocarbons in liquid condition at the specified temperature (-150°C) and pressure (145 psia).

The following are specified for the refrigerator design:

- Use of MR to better match cooling curves
- Use of a multistage/cascade process to reach cryogenic temperatures
- Use of a coil-wound heat exchanger for heat transfer.

Cryogenic Refrigeration Cycle

The ENDP product stream leaving Compressor 2 is cooled first by cooling water to 1°C. Then the refrigeration system is responsible for further cooling the stream to a temperature that makes feasible cryogenic distillation. This system envisions a three-step cascade process using phase separators, throttle valves (Joule-Thomson [JT] valves), and coil-wound heat exchangers.

In general, a traditional liquefaction cycle is composed of several heat exchangers, JT valves, and vapor-liquid phase separators, as shown in Figure H - 1. Pressurized MR in the compressor is separated to vapor and liquid by the first-phase separator. Liquid refrigerant is expanded and cooled down by the first JT valve, and it cools down the already-separated vapor refrigerant and natural gas by passing through the heat exchanger, then goes back to the compressor. Vapor refrigerant is cooled by the liquid refrigerant and goes to the second phase separator.

The separated liquid refrigerant from the second phase separator is expanded again by the second JT valve and goes back to the compressor after cooling down the vapor refrigerant and natural-gas stream simultaneously. Finally, the vapor refrigerant from the second phase separator is expanded at the third JT valve and liquefies the natural gas. Cold exergy from the coldest refrigerant is regenerated consecutively by heat exchangers. Use of JT valves always generates entropy due to their intrinsic irreversibility.

The specific composition of refrigerant is determined with two constraints. First is to have low enough product temperature, and the other is the reasonable compressor inlet temperature of MR. The compressor inlet should have higher temperature than 273 K to have realistic simulation results. The composition that can have the lowest product temperature has been chosen for each processes. For the MR-JT cycle, the composition was selected as C1:C2:C3=0.4:0.2:0.4 (or C1:C3:N2 = 0.35:0.45:0.2). It was the best composition to have the lowest product temperature

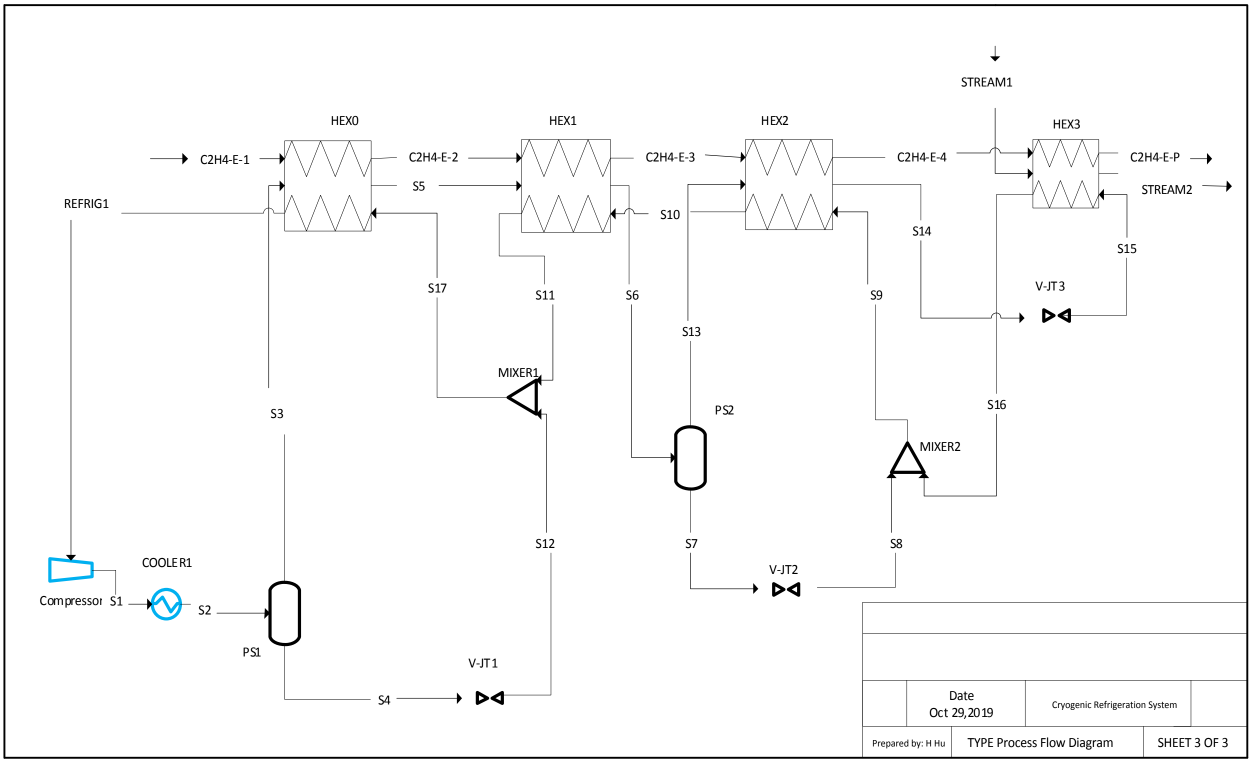


Figure H - 1. Schematic diagram of general MR-JT (mixed refrigerant-JT valve) liquefaction cycle.

Refrigeration Unit Efficiency

Energy enters the system in the form of shaft work for the compressor-turbine system power (work of compressor). Energy exits the system in the form of cooling duties. The coefficient of performance (COP) can be determined using the values of power and cooling duties determined above. Equation (H1) is used to determine the COP.

$$\text{COP} = Q(\text{cooling duty})/W\ (\text{compressors}) \tag{H1}$$

A COP of 30% is commonly applied in industries.

Appendix I

Cost Information

Appendix I

Cost Information

Capital costs of equipment were derived from four sources:

1. Aspen Economic Analyzer
2. Lindgren Group Report (2013) on "Production of Ethylene from Natural Gas"
3. Petrochemical Update 2018, "US Ethylene complex construction costs data 2018–2020"
4. The H2A model.

Table I - 1. Capital cost list for equipment for ENDP current case.

Name		**Equipment Cost [$]**
Mixer1	Valve Mixing	5,000
Compres1	1 Stage	7,275,300
Mixer2	Valve Mixing	5,000
NUHEAT	Heat Exchanger	1,520,200
Hex1	Heat Exchanger	2,518,900
Hex3	Heat Exchanger	1,763,230
Expander	Expander	137,413
ENDP Reactor	Electrochemical Reactor	71,787,195
ENDP Reactor BOP	BOP for ENDP	83,074,721
Cooler0	Cooler	493,300
Compres2	Compressor	20,757,800
Cooler1	Cooler	174,800
Compres3	Compressor	4,715,100
Cooler2	Cooler	105,500
Membrane Separation		
HEX2	Heat Exchanger	12,800
CH_4SEP	Membrane Separation for CH_4	2,900,000
H_2N_2SEP	Membrane Separation for H_2/N_2	2,900,000
(including Compress4)		

C_2H_4SEP	Membrane Separation For C_2H_4/C_2H_6	
(including Compress5)		50,000,000
Distillation Columns		
Heater2	Heater	32,900
Cooler3	Cooler	19,200
Cooler4	Cooler	25,600
Ch4h2sep	Distillation Column	5,034,680
C2seplt	Distillation Column	7,192,400
C3c4splt	Distillation Column	270,100
C3splt	Distillation Column	569,800
COLDBOX	Refrigeration System	16,598,147
Total Uninstalled Equipment Cost		**279,889,086**

Table I - 2. Capital cost list for equipment for ENDP future case.

Name		**Equipment Cost [$]**
Mixer1	Valve Mixing	5000
Compres1	1 Stage	7275300
Mixer2	Valve Mixing	0
NUHEAT	Heat Exchanger	720300
Hex1	Heat Exchanger	716700
Hex3	Heat Exchanger	33400
Expander	Expander	597600
ENDP Reactor	Electrochemical Reactor	37,644,504
ENDP Reactor BOP	BOP For ENDP	43,563,573
Cooler0	Cooler	208900
Compres2	Compressor	9414700
Cooler1	Cooler	92000
Compres3	Compressor	2735800
Cooler2	Cooler	58700

Membrane Separation		
Hex2	Heat Exchanger	12,800
Ch_4sep	Membrane Separation for CH_4	2,900,000
H_2N_2sep	Membrane Separation for H_2/N_2	2,900,000
(Including Compress4)		
C_2H_4sep	Membrane Separation for C_2H_4/C_2H_6	
(Including Compress5)		34,860,956
Distillation Columns		
Heater2	Heater	19500
Cooler3	Cooler	12800
Cooler4	Cooler	21900
Ch4h2sep	Distillation Column	575750
C2seplt	Distillation Column	822,500
C3c4splt	Distillation Column	232,200
C3splt	Distillation Column	515,900
COLDBOX	Refrigeration System	10,458,290
Total uninstalled equipment cost		156,399,073

Table I - 3. Detailed direct operation costs for steam cracking process.

Section	**Unit operation**	**Type of Utility Used**	**$/tonne ethylene**
Pyrolysis	Feedstock Preheater	CH_4	30
	Cracker	CH_4	32
	Transfer line exchanger	Cooling Water	8
Compression	Recirculation Heater	Cooling Water	6
	Interstage cooler	Cooling Water	4
Separation	Cool train	Refrigerant	21
	Reboiler	Steam	38
	Condenser	Refrigerant	56

	Acetylene Preheater	Steam	11
Total Thermal Energy			205
Compression	Compressor	Power	46
Feedstock Ethane		NG Liquid	235
Labor			36
Total Direct Cost			521

Table I - 4. Detailed direct operation costs for ENDP process.

	Unit Operation	**Type of Utility Used**	**Current**	**Future**	**Current**	**Future**
			MMBTUs/tonne		**$/tonne**	
	ENDP Thermal	CH_4	6.532	4.681	26.13	18.73
	Feedstock Preheater	NPP low steam	3.543	0.630		
Thermal	Reboilers	NPP Low Steam	3.153	1.081		
	Preheater1	Steam	0.053	0.036		
	Preheater2	Steam	0.779	0.226		
	Subtotal		**14.061**	**6.654**	76.20	19.96
Cooling	Interstage Cooler	Cooling Water	1.665	0.547		
	Condersors (3rd/4th)	Cooling Water	0.779	0.428		
	Separation Coolers	Cooling Water	0.159	0.059		
	Subtotal		**2.604**	**1.034**	5.21	2.07
Refrigeration	COLDBOX Refrigiration	Refrigerant	5.421	1.521		
	Condersors (1st/2nd)	Refrigerant	1.949	0.594		
	Subtotal		**7.370**	**2.115**	147.39	42.30
	ENDP Electricity	Electricity	0.891	0.891		
Reaction and Compressor	Feed Compressor1	Electricity	0.175	0.117		
	Expander	Electricity	-0.355	-0.041		
	Cooling Compressor	Electricity	1.533	0.511		
	COLDBOX Compressors	Electricity	10.842	5.069		
	Membrane Compress4	Electricity	0.092	0.059		
	Electricity Subtotal		**13.178**	**6.607**	115.87	58.09
	Non-Electricity		24.035	9.803		

	Subtotal					
Ethane					372.00	263.77
Labor					28.69	6.78
Total					771.48	411.69

Cash Flow and Net Present Value

To assess the IRR and NPV of each scenario, it is necessary to calculate the after-tax cash flow (ATCF). To calculate the ATCF it is necessary to first calculate the revenues (R_k); cash outflows (E_k); sum of all noncash, or book, costs such as depreciation (d_k); net income before taxes; the effective income tax rate (t); and the income taxes (T_k), for each year (k). The taxable income is revenue minus the sum of all cash outflow and noncash costs. Therefore, income taxes per year are defined as follows (Turton 2010, Wood 2010):

$$T_k = t\,(R_k - E_k - d_k) \qquad (1)$$

Depreciation for the economic calculations was calculated using a standard MACRS depreciation method with a property class of 5.5 years (Turton et al. 2010).

The ATCF is then the sum of the before tax cash flow (BTCF) minus the income taxes owed. Note that the expenditures for capital are not taxed but are included in the BTCF each year there is a capital expenditure (C_k); this includes the equity capital and the debt principle. The BTCF is defined as follows (Turton 2010):

$$BTCF_k = R_k - E_k - C_k \qquad (2)$$

The ATCF can then be defined as:

$$ATCF_k = BTCF_k - T_k \qquad (3)$$

Discounted Cash-Flow Rate of Return or Internal Rate of Return

The IRR method is the most widely used rate of return method for performing engineering economic analyses. This method solves for the interest rate that equates the equivalent worth of an alternative’s cash inflows to the equivalent worth of cash outflows (ATCF)—i.e., the interest rate at which the NPV is zero. The resulting interest is the IRR (i'). For the project to be economically viable, the calculated IRR must be greater than the desired minimum annual rate of return (Wood 2010, Turton 2010).

$$NPR(i'\,\%) = = 0 \qquad (4)$$

IRR calculations were performed for a 60:40 debt-to-equity ratio for the calculated TCI and at low, average, and high product-ethylene prices. The IRR and product price required (for an IRR of 12%) was solved for using the Goal Seek function in Excel.