AVEVA Academic Competition 2023 – Part 1 Submission

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This document presents the required deliverables specified in the problem description part 1. Simulations for PEM electrolysis and ammonia synthesis are combined into a single .simx file, contained in "PEM_Electrolysis" and "Main" flowsheet, respectively. All the necessary calculations (thicknesses, SPC, etc.) were carried out using flowsheet equations in APS—most of the contents presented in this document are directly accessible in the submitted simulation file.

1. Stream Table from the simulation (Table 1)

The reference data given in the problem description is presented in Table 2 for a comparison.

Table 1. Simulation result obtained from the .simx file

Stream no.	1	2	3	4	5	6	7	8	9	10	11
Model name in APS	S1	S2	S4	S5	S6	S8	S13	S22	S19	S24	S17
Temperature [°C]	80.00	307.96	270.80	25.00	217.50	313.60	430.44	50	297.31	50.63	33.86
Pressure [bar]	8.9	35.6	150	7	28	150	149.3	149.2	150	150	17.24
Vapor fraction	1	1	1	1	1	1	1	1	1	1	0
Mass flow [kg/h]	21,745	21,745	21,745	101,446	101,446	101,446	1,935,029	9,035	13,889	1,797,949	114,155
Mole flow [kmol/h]	10,787	10,787	10,787	3,614	3,614	3,614	170,919	817	898	162,500	6,705
Mole fraction											
Hydrogen	1	1	1	0	0	0	0.5448	0.5693	0.1545	0.5693	0.0005
Nitrogen	0	0	0	0.995	0.995	0.995	0.1818	0.1900	0.0445	0.1900	0.0001
Ammonia	0	0	0	0	0	0	0.2527	0.2191	0.7895	0.2191	0.9993
Argon	0	0	0	0.005	0.005	0.005	0.0207	0.0216	0.0115	0.0216	0.0001

Table 2. Reference data given in the problem description

Stream no.	1	2	3	4	5	6	7	8	9	10	11
Temperature [°C]	80	308	270.8	25	217.5	313.6	430.4	50	296.9	50.6	34
Pressure [bar]	8.9	35.6	150	7	28	150	149.3	149.2	150	150	17.24
Vapor fraction	1	1	1	1	1	1	1	1	1	1	0
Mass flow [kg/h]	21,740	21,740	21,740	101,426	101,426	101,426	1,930,310	9,012	13,827	1,793,316	114,155
Mole flow [kmol/h]	10,785	10,785	10,785	3,613	3,613	3,613	170,471	814	894	162,058	6,705
Mole fraction											
Hydrogen	1	1	1	0	0	0	0.5447	0.5693	0.155	0.5693	0.0005
Nitrogen	0	0	0	0.995	0.995	0.995	0.1818	0.19	0.0447	0.19	0.0001
Ammonia	0	0	0	0	0	0	0.2528	0.2191	0.7888	0.2191	0.9993
Argon	0	0	0	0.005	0.005	0.005	0.0207	0.0216	0.0115	0.0216	0.0001

2. The number of solar arrays and total area of those arrays required to produce the desired amount of 114,155.25 kg/h of ammonia

Number of arrays:	4348	arrays
Total area of the solar farm:	9,844,014	m^2

3. Reactor and vessel thicknesses

Reactor thickness:	0.418	m
LP flash vessel thickness:	0.111	m
HP flash thickness:	0.012	m

4. Single pass conversion (SPC) of hydrogen to ammonia in the reactor

SPC:	9.976	%

5. Suggestions for optimization

Firstly, the compression ratios of two compressors for each feed can be optimized to minimize the total electrical duty of the process while maintaining the same final pressure.

Secondly, the main process variables in the reactor, namely the temperature and pressure, could be optimized. Too low a temperature would slow down the reaction, therefore higher tau would be mandated to reach an equilibrium in the reactor (which might not be visible on the simulation since a Gibbs reactor model is used, not a kinetic model), while too high a temperature would penalize the thermodynamics, lowering the SPC. The highest achievable temperature is limited by available heating utilities as well as material constraints.

Regarding pressure, change in the reactor pressure would also shift the thermodynamic equilibrium in the reactor and affect the overall power demand. Through optimization, the pressure that minimizes the total power demand (or capital and operating costs) per unit mass of ammonia produced could be determined.

In addition, the operating pressures of high- and low-pressure flash vessels could be adjusted to either maximize the sharpness of the separation or achieve the lowest production cost while meeting a desired quality standard.

Because the product exiting the reactor is at a very high temperature and needs to be cooled down for separation of ammonia, its heat can be used in the feed preheating process, which would reduce costs for both heating and cooling utilities. This can be done by allowing a heat exchange between the cold feed (67 °C) and the hot product (430.4 °C) streams.

SRK EOS was chosen as the thermodynamic model for this simulation to match the information provided in the problem description. However, a comparative study on the accuracy of other available thermodynamic models with available experimental data in the operating range of the process would help to justify the selection.

AVEVA Academic Competition 2023 – Part 2 Submission

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2024-01-02

This document includes the required deliverables specified in the problem description part 2. The base case has been optimized to maximize the net present value (NPV) of the process. All necessary calculations (thicknesses, SPC, reactor's space time) were carried out using flowsheet equations in AVEVA™ Process Simulation (APS).

1. A screenshot of the flowsheet for the optimized Ammonia process design.

The flowsheet of the optimized process is presented in Figure 1. The blue connections represent cooling water streams and the red connections heating streams (HP steam, LP steam, and hot circulating oil) in the flowsheet.

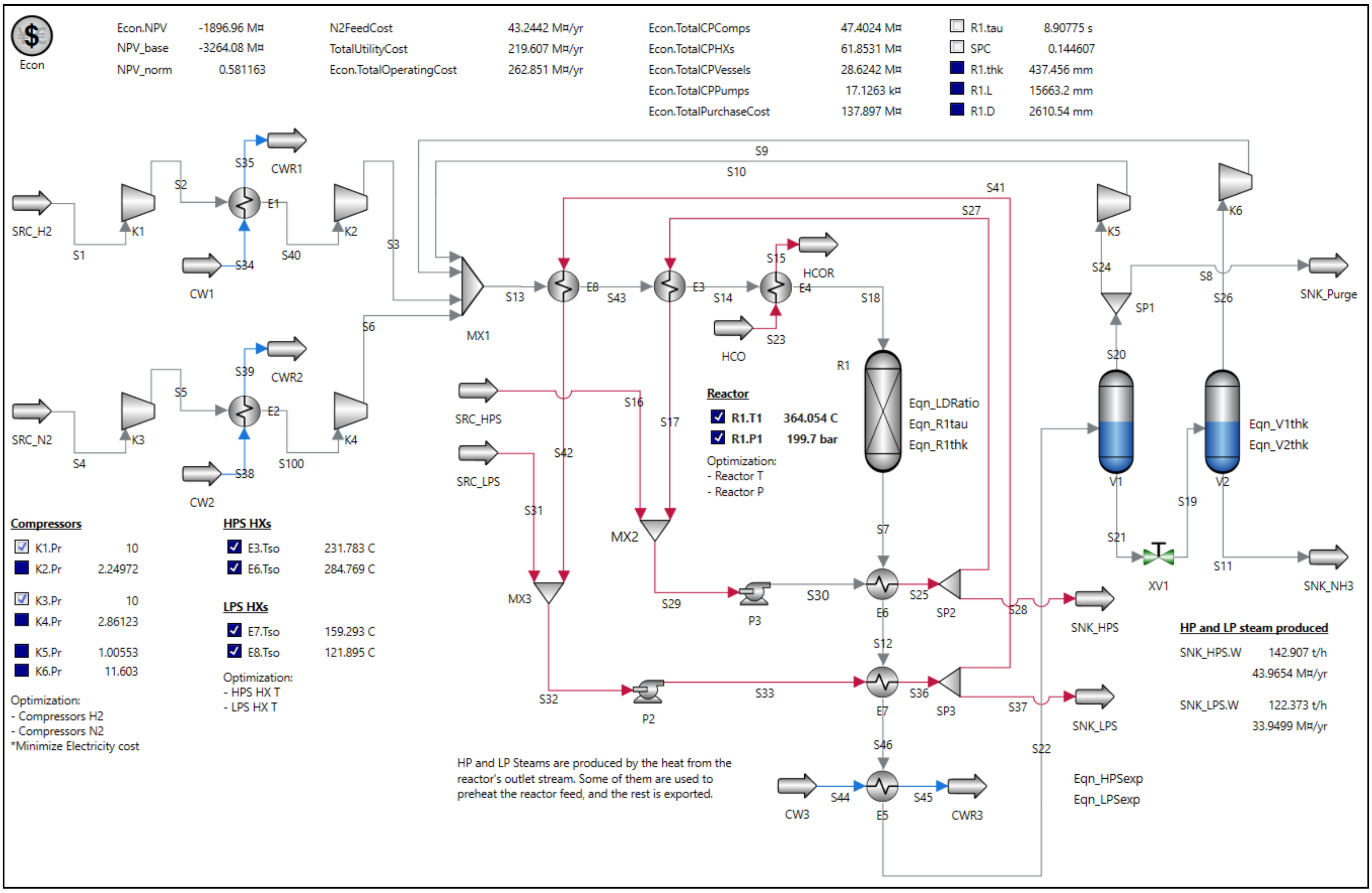

Figure 1. The flowsheet of the optimized process.

2. An updated table of the streams (Table 1).

Information of important streams in the process are summarized in Table 1.

Table 1. Simulation result obtained from the optimized process.

Stream no.	1	2	3	4	5	6	7	8	9	10	11
Model name in APS	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11
Temperature [°C]	80.00	313.27	321.72	25.00	299.44	280.10	458.65	50.00	339.81	50.65	32.44
Pressure [bar]	8.90	36.56	200.0	7.0	44.48	200.00	199.20	198.90	200.00	200	17.24
Vapor fraction	1	1	1	1	1	1	1	1	1	1	0
Mass flow [kg/h]	21,163	21,163	21,163	98,731	98,731	98,731	1,278,610	5,738	16,767	1,141,949	114,155
Mole flow [kmol/h]	10,498	10,498	10,498	3,517	3,517	3,517	110,679	514	1,090	102,370	6,704
Mole fraction											
Hydrogen	1	1	1	0	0	0	0.5448	0.5842	0.1746	0.5842	0.0005
Nitrogen	0	0	0	0.995	0.995	0.995	0.1820	0.1952	0.0494	0.1952	0.0001
Ammonia	0	0	0	0	0	0	0.2425	0.1877	0.7573	0.1877	0.9992
Argon	0	0	0	0.005	0.005	0.005	0.0307	0.0328	0.0187	0.0328	0.0001

3. A converged simx file for the optimized ammonia synthesis process

The file "Part 2 submission Seonggyun Kim.simx" was submitted together with this document.

4. An economic summary

Consumed or produced utilities and cost of each type of the utilities in the optimized process and the base case are presented together in Table 2. The base case uses high-pressure steam (HPS) as a heating medium, however, in the optimized process, high- and low-pressure steam are net produced. The net operating cost is calculated by deducting the product value of produced steam from the total operating cost. It is noted that the cost of the feed nitrogen was not considered in Table 2. Steam products that only exist in the optimized process are denoted with an asterisk (*).

Table 2. Economic summary: consumed or produced utilities in optimized and the base case.

Utility	Optimized			Base case		
	Consumption		**Cost [M$/yr]**	**Consumption**		**Cost [M$/yr]**
Cooling water	15461.90	m3/h	11.75	59013.80	m3/h	44.83
HP Steam		-	-	639.00	t/h	196.59
Hot circulating oil	4674.46	t/h	111.79	6422.22	t/h	153.59
Electricity	62.59	MW	88.74	56.75	MW	80.47
	Production		**Value [M$/yr]**	**Production**		**Value [M$/yr]**
*HP Steam	142.91	t/h	43.97	-		-
*LP Steam	149.61	t/h	41.51	-		-
Total utility cost [M$/yr]			212.27			475.48
Net utility cost [M$/yr]			126.80			

Table 3 shows all equipment in the optimized process and the base case. Similarly to Table 2, equipment that were added to the base case are denoted with an asterisk (*).

Table 3. Economic summary: Equipment purchase cost.

	Equipment	**Description**	**Purchase Cost [$]**	
			Optimized	**Base Case**
Compressors	K1	1st H2 compressor	15,850,519	15,893,849
	K2	2nd H2 compressor	17,732,989	15,767,202
	K3	1st N2 compressor	3,538,104	2,866,120
	K4	2nd N2 compressor	3,252,911	3,571,250
	K5	HP recycle compressor	1,705,770	2,191,338
	K6	LP recycle compressor	4,985,516	3,950,181
Heat Exchangers	E1	H2 feed intercooler	661,656	670,323
	E2	N2 feed intercooler	76,123	65,364
	E3	Feed preheater (HPS)	5,466,952	15,881,835
	E4	Feed preheater (HCO)	14,797,899	19,502,624
	E5	Product cooler	23,751,651	43,974,321
	*E6	HPS production	5,706,349	-
	*E7	LPS production	7,606,498	-
	*E8	Feed preheater (LPS)	2,841,077	-
Reactor/Vessels	R1	Ammonia synthesis reactor	27,265,267	26,737,454
	V1	HP separation vessel	1,298,001	1,023,348
	V2	LP separation vessel	31,233	31,215
*Pumps	*P1	HPS pump	9,959	-
	*P2	LPS pump	7,169	-
Total Purchase Cost [M$]			136.59	152.13

5. Approach

Initial setup

First, to accurately reflect the effects of process variables on the capital investment and operating costs, economic submodels were added to the existing models. Stainless steel 304 was chosen as the material for equipment in contact with hydrogen and carbon steel was chosen for the rest (cast iron was chosen when carbon steel was not available). In addition, a flowsheet equation was added to express the reactor's space time (R1.tau) as an exponential function of the reactor's inlet temperature. Finally, the NPV of the base case was recorded as a reference throughout the optimization process.

Heat recovery by LPS and HPS streams

From the base case, I noticed the possibility of recovering the heat from the reactor's product stream (S7) to preheat the reactor's inlet feed stream (S13 to S18). However, a direct heat exchange of the two streams would mandate a very expensive heat exchanger because of the low overall heat exchange coefficient of gas-gas heat exchange. Therefore, I decided to introduce low- and high-pressure steam as heating/cooling media that have much higher heat exchange coefficient. Because the cooling demand is greater than the heating demand in the process, excess steam produced by the hot product stream can be exported. I added "Product" submodels to the excess steam sink models to calculate the product value using the same price as given in the economic summary model. Integrating the heat recovery system resulted in lowering both cooling and heating demand, effectively reducing purchased costs as well as operating costs.

It was assumed that saturated liquid condensates at the same pressure as the used condensates are available. TEFC (total enclosed, fan-cooled) enclosure electric drivers were chosen for the pumps.

The reactor inlet P/T and the heat exchangers' outlet T

I used case studies to observe how NPV behaves as a function of each of process variables, such as the reactor's inlet temperature and pressure (R1.T1 and R1.P1), the heat exchangers' outlet temperatures, etc. For the reactor's inlet pressure, no optimum was found in the range of 150–200 bar, with NPV being highest at 200 bar (199.7 bar at the reactor inlet due to pressure drops in the preheaters). This is largely due to the shift of equilibrium that increases the overall efficiency of the process.

For the reactor inlet temperature and shell-side outlet temperatures of the steam heat exchangers (E3, E6, E7, E8), a clear optimum was observed in the case studies. Then I proceeded to use optimization sets to set the variables to the optimum and verified that there is enough temperature difference to drive the heat exchange in each exchanger.

Feed compressors

A case study showed that when the NPV is the objective function and the pressure ratios of the feed compressors are variables, the optimization curve appears pretty much linear, preferring lowest possible pressure ratios in the first compressors (K1 and K3). This is because the purchase cost is the lowest when one of the compressors has a pressure ratio of 1 (which is similar to having just one compressor instead of two), according to the calculations by "CapExComp" submodels. However, in real applications, it is common to avoid putting all the compression load to a single compressor because of high temperature of the compressed gas and material constraints. Therefore, instead of NPV, total electricity cost (calculated by the economic summary model) was chosen as the objective function (to maximize) when optimizing the feed compressors.

AVEVA Academic Competition 2023 – Part 3 Submission

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This document includes the required deliverables specified in the problem description part 3.

1. A screenshot of the flowsheet for the optimized hydrogen pipeline design.

The flowsheet of the optimized pipeline is presented in Figure 1.

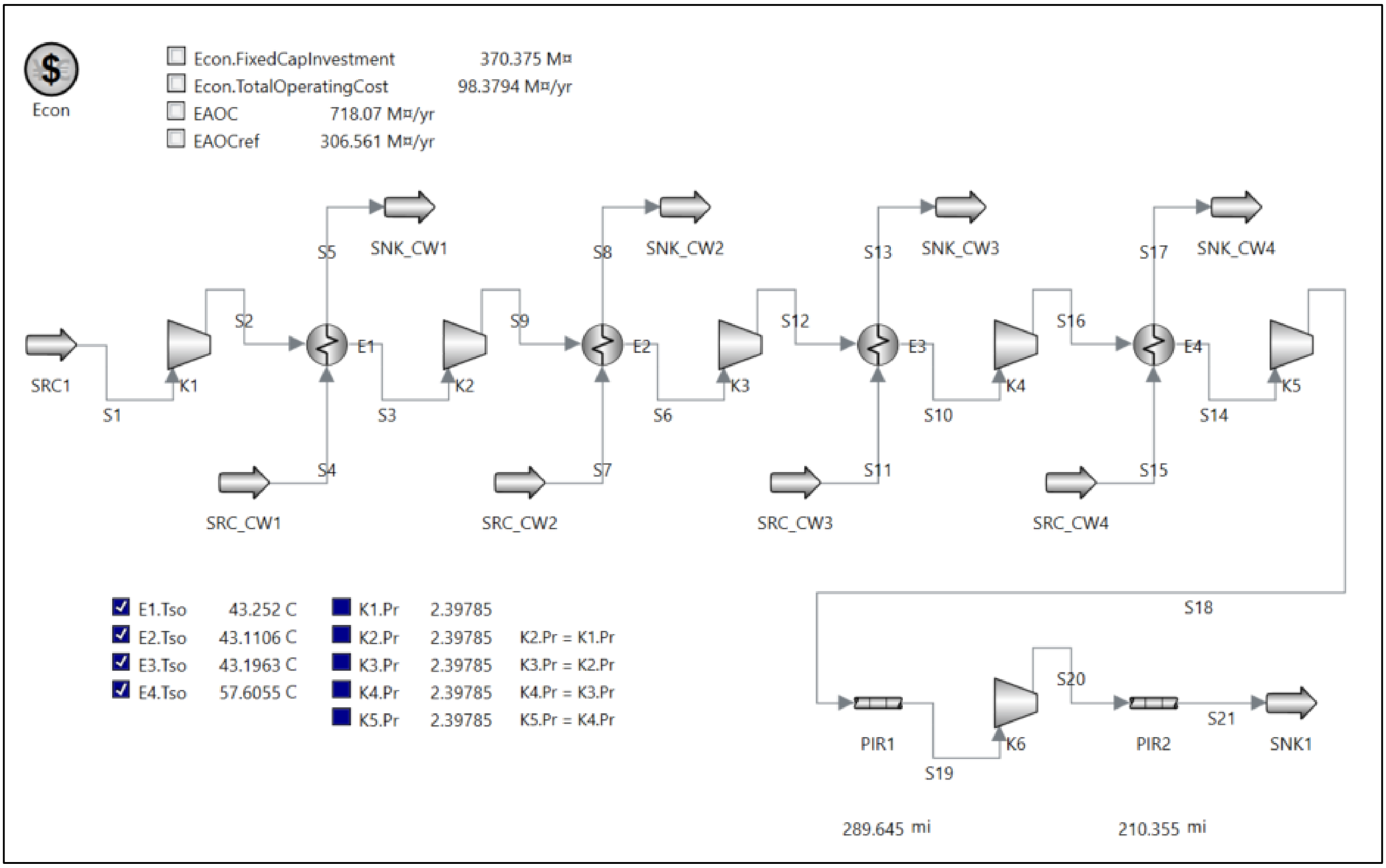

Figure 1. The flowsheet of the optimized pipeline.

2. A converged simx file for the optimized ammonia synthesis process

The file "Part 3 submission Seonggyun Kim.simx" was submitted together with this document.

3. An economic summary

Consumed amounts and costs for cooling water and electricity in the process are summarized in Table 1.

Table 1. Economic summary: consumed utilities in the optimized pipeline system.

Utility	Consumption		Cost [M$/yr]
Cooling water			
CW1	0.3570	m^3/hr	0.98
CW2	0.2534		0.69
CW3	0.2561		0.70
CW4	0.2318		0.63
	1.0982		3.00
Electricity			
K1	11.72	MW	16.63
K2	10.62		15.06
K3	10.86		15.40
K4	11.49		16.29
K5	13.58		19.25
K6	8.99		12.74
	67.26		95.38
Total Utility Cost			98.38

Table 2 shows all equipment and respective purchases costs in the process.

Table 2. Economic summary: Equipment purchase cost.

	Equipment	Description	Purchase Cost [M$]
Compressors	K1	Compression stage 1	11.32
	K2	Compression stage 2	10.63
	K3	Compression stage 3	10.78
	K4	Compression stage 4	11.17
	K5	Compression stage 5	12.41
	K6	Booster compressor station	9.57
Heat Exchangers	E1	Intercooling b/w K1 and K2	0.45
	E2	Intercooling b/w K2 and K3	0.66
	E3	Intercooling b/w K3 and K4	1.01
	E4	Intercooling b/w K4 and K5	1.97
Pipeline	PIR1	1st Segment	1939.39
	PIR2	2nd Segment	1408.38
		Total Purchase Cost [M$]	3417.76

4. Equivalent annual operating costs (EAOCs) of the optimized pipeline and the ammonia plant

The EAOCs of the ammonia process and the hydrogen pipeline were calculated using flowsheet equations in APS.

The EAOC of the ammonia process that I have optimized in Part 2 of the competition is 306.56 M$/yr, considering the product value of steams generated in the process and assuming we use already existing pipelines for transportation and distribution of the produced ammonia.

The EAOC of the hydrogen pipeline optimized in Part 3 is 718.07 M$/yr.

5. Approach

First, I introduced a five-stage compression process with intercoolers, limiting the single-stage compression ratio for hydrogen under 2.5. After adding Economics submodels and flowsheet equations that calculate the EAOC of the pipeline system, the outlet temperature of hydrogen from each of the intercooling heat exchangers was optimized to minimize the EAOC. I assumed all the compressors share the same compression ratio, which is 2.40.

Following the compression process, I added two pipeline models separated by a booster compressor. Here, I focused on three variables: pressure drop of the two pipeline models (determining their diameters) and the position of the booster compression station. I first observed effects of varying these variables using case studies, then proceeded to make an optimization set to find a set of these three variables that minimizes the EAOC of the process. At the optimum, the booster compression station is approximately 290 miles away from the starting point, the pressure drops of the pipeline models were 326 and 220 bar respectively, and diameters of both pipeline segments were approximately 7 inches. The pipeline optimization reduced the EAOC by approximately 50 M$/yr compared to my initial arbitrary base case, where the booster station was placed right in the middle and the pipeline models had 100 bar pressure drop each.

The pressure drop of the second segment of the pipeline (PIR2) is not necessarily an optimum value, because it is limited by the upper bound of the pressure of the fluid model, which is 700 bar. Although better optimization results might have been available if a higher pressure range was explored, I decided to limit the maximum pressure of hydrogen at 700 bar based on current data of existing industrial-scale hydrogen pipelines and the difficulties in compressing hydrogen.