OCT 15TH, 2024

Modelling an Ammonia Synthesis Process for Hydrogen Economy on APS

APS Academic Competition 2024

Presented by Seonggyun Kim

AVEVA

Overview of the project

- AVEVA Process Simulation (APS) 2023.2 version has been used
- 5 Tutorial videos to guide through each function of APS
- Objective
  - To produce 21,740 kg/h of hydrogen from solar panels and convert them to ammonia product with 114,155.25kg/h mass flow rate
- Part 1 – Simulation building (Nov 1st, 2023 - Dec 1st, 2023)
- Part 2 – Simulation optimization (Dec 4th, 2023 – Jan 2nd, 2024)
- Part 3 – Pipeline implementation (Jan 3rd, 2024 – Feb 2nd, 2024)

Introduction

Background information

- Why Hydrogen fuel?
- Method for conversion to ammonia
- Reversible reaction
  - Forward reaction is exothermic
- Favored high pressure and low temperature
- Typical single-pass conversion is 10%
- Using adiabatic Gibbs free reactor

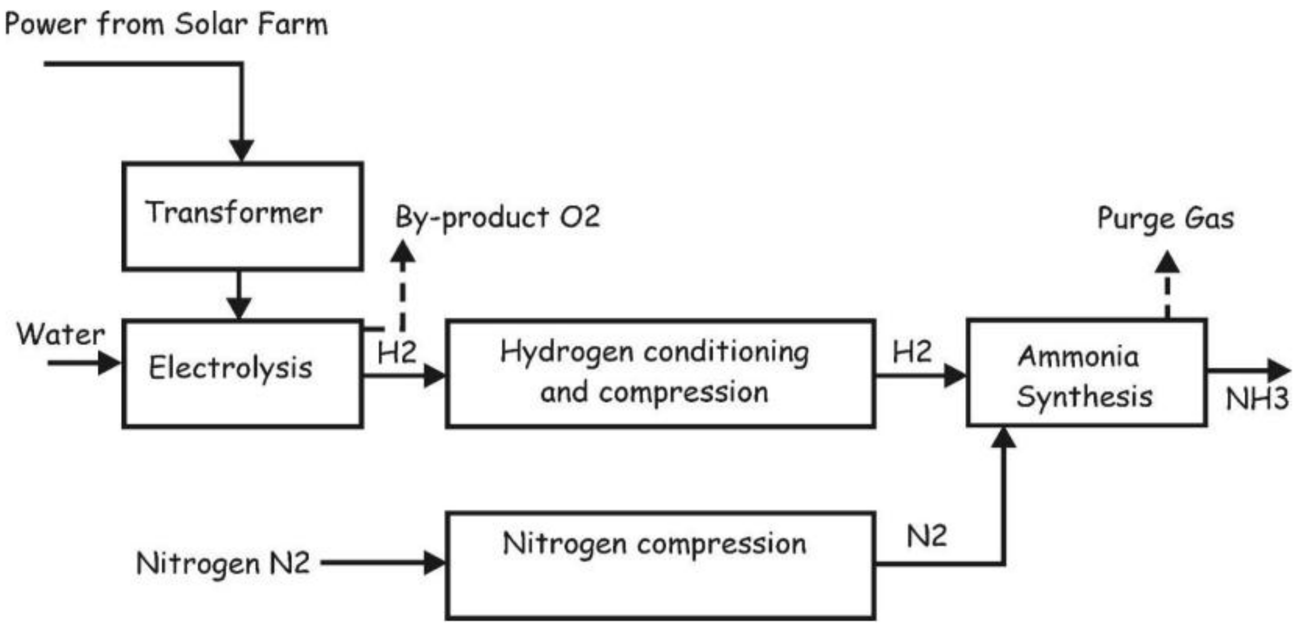

Figure 1: Block flow diagram for production and transportation of ammonia from hydrogen

Introduction – Part 1

Process design

- Deliverables:
  - Number of solar panel arrays needed to produce ammonia at 1,000,000 tonne/y
  - Thickness of the vessel
  - The single pass-conversion of hydrogen to ammonia
  - Idea for optimization

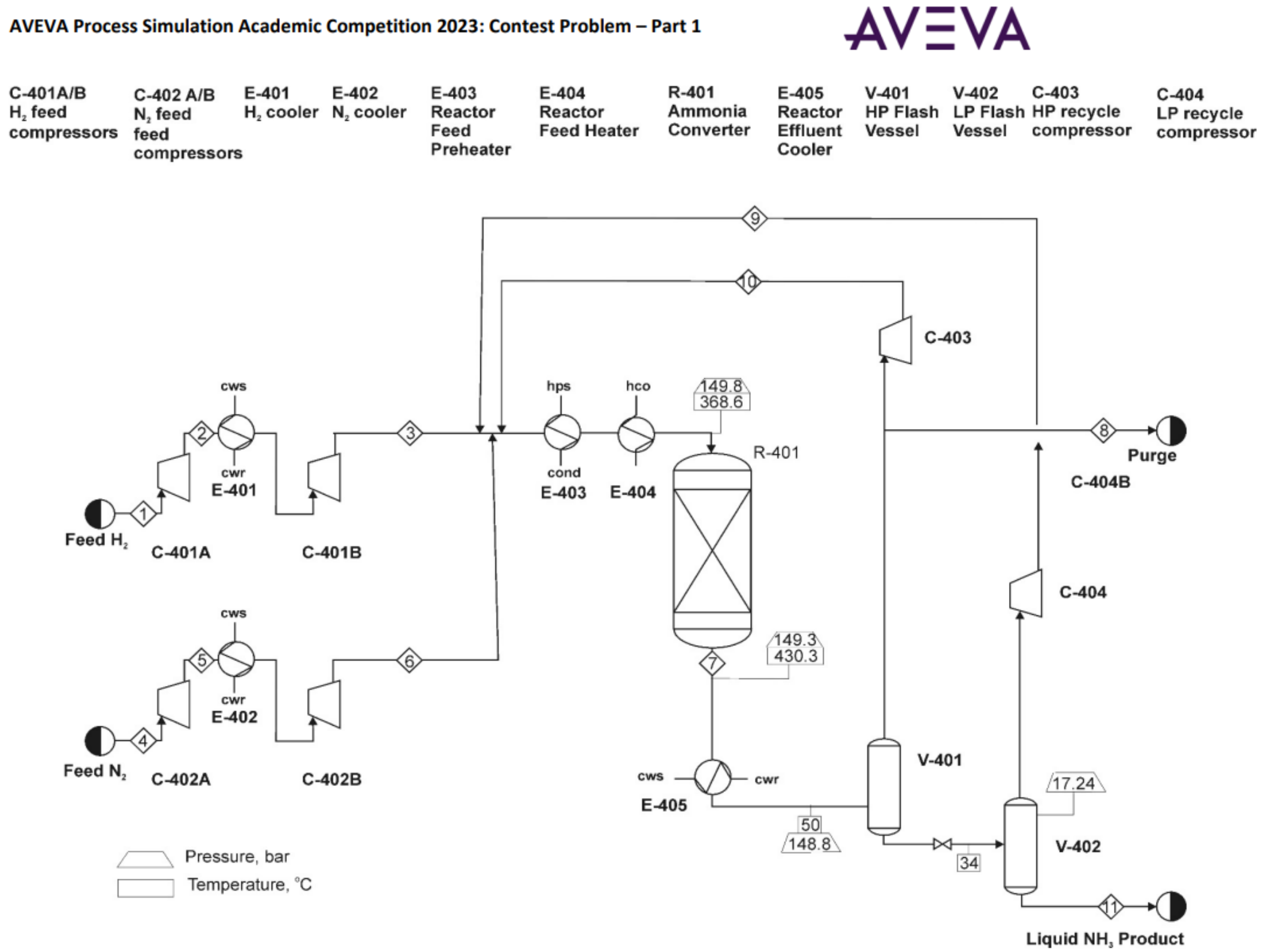

Figure 2: Preliminary Process Flow Diagram for Ammonia Synthesis Plant

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Introduction – Part 2

Process optimization

- Base simulation was given for normalization
- Objective function: Net Present Value (NPV) in *Economic Summary* model
  - Negative value, since the value of product ammonia is not taken into account.
- *RawMatl*, *CapEx*, *Utilitiy* submodels to calculate equipment purchase cost

- Adiabatic Gibbs reactor (*GMR*)
  - Temperature: 350 – 400 °C
  - Pressure: 150 – 200 bar
- Available utilities
  - Cooling water
  - Low-, medium-, and high-pressure steam
  - Hot oil
- Material constraints
- Overall heat transfer coefficients given for different configurations

  a. Gas - Gas U = 100 W/m2/K
  b. Gas - Liquid U = 200 W/m2/K
  c. Liquid-Liquid U = 500 W/m2/K
  d. Gas - condensing vapor or boiling liquid U = 500 W/m2/K
  e. Liquid - condensing Vapor U = 1000 W/m2/K

Introduction – Part 3

Hydrogen pipeline

- Direct transportation of pressurized hydrogen over a 500-mile pipeline
- Rigorous pipe model (*PipRig*) to be used
- Minimize Equivalent Annual Operating Cost (EAOC) planned for 6 years
- Pipeline cost calculation

The cost of a new H_2 pipeline is given by the following equation:

$$\text{Installed Pipeline Cost [\$/mile]} = 5\times10^6 + 1.5\times10^6(D\ [\text{inch}]/6)^{0.7}$$

Where *D* is the pipe diameter in inches. For example, a 3-inch pipe, costs $\$(5+1.5(3/6)^{0.7}) =$ \$5.92 million for 1 mile of pipeline. Note that the diameter of pipeline should not be less than 1-inch.

- One or more booster compressors may be installed along the pipeline

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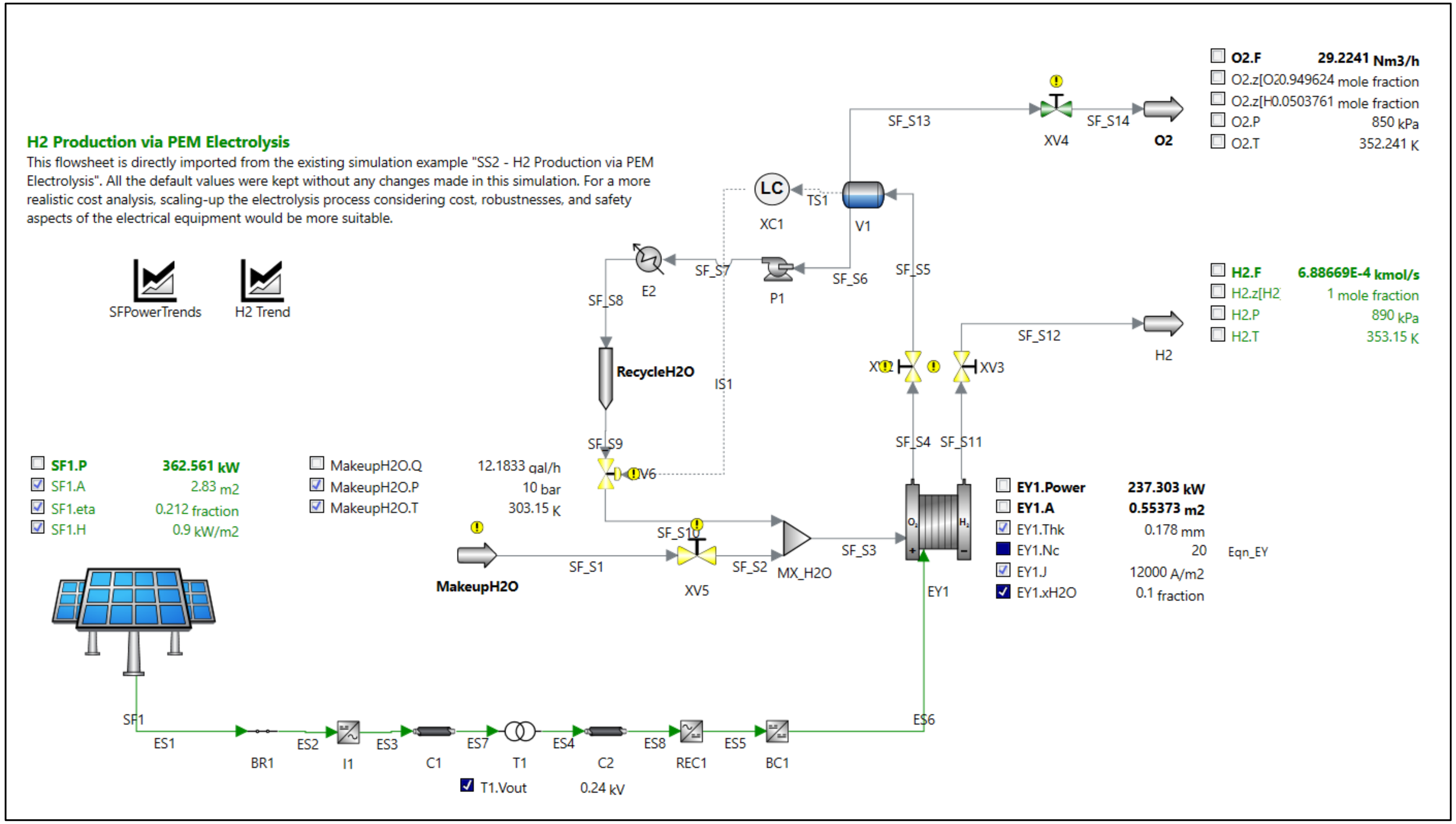
Part 1 – Simulation Building

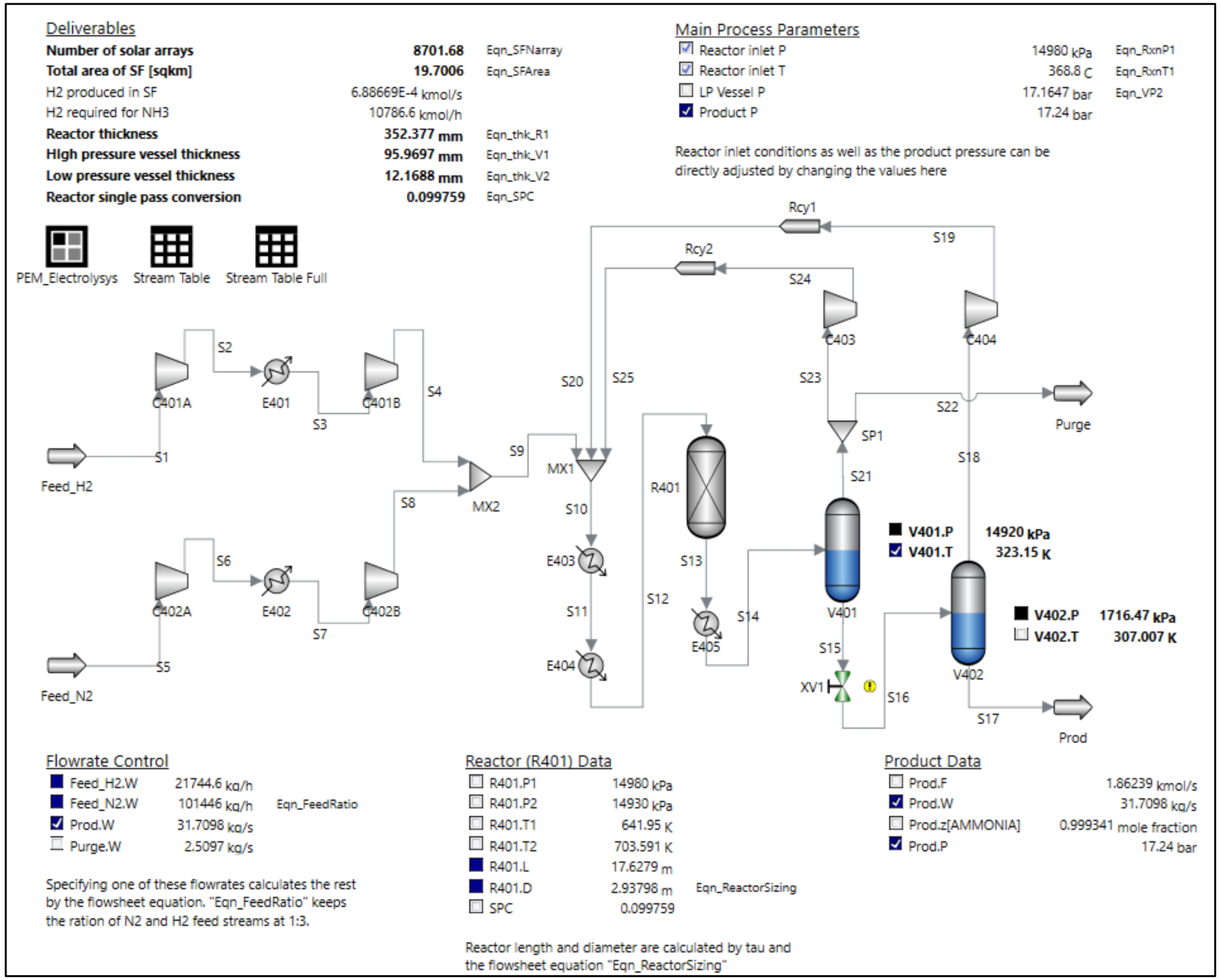
PEM Electrolysis



- Simple scale-up by a factor of 8700 to produce enough H2
- For a more realistic cost analysis, scaling up the electrolysis process considering cost, robustness, and safety aspects of the electrical equipment would be more suitable.

Part 1 – Simulation Building

PEM Electrolysis



- Flowsheet equations to calculate:
  - solar farm area
  - reactor/vessel thicknesses
  - single pass conversion
- Variable references to monitor/specify different process parameters

Part 1 – Simulation Building

Stream table

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

- Obtained stream properties/composition matched the reference data almost exactly.

Part 1 – Simulation Building

Suggestions for optimization

- Compressors
  - Adjust compression ratios to reduce power use while keeping final pressure.
- Reactor
  - Temperature: Balance to avoid slow reactions or thermodynamic penalties.
  - Pressure: Optimize for minimal power demand or cost.
- Flash Vessels
  - Tune pressures for better separation or lower costs.
- Heat Integration
  - Use reactor heat to preheat feed, saving on utilities.
    - ~500 MW heating from 68 to 368 °C
    - ~660 MW cooling from 430 to 50 °C

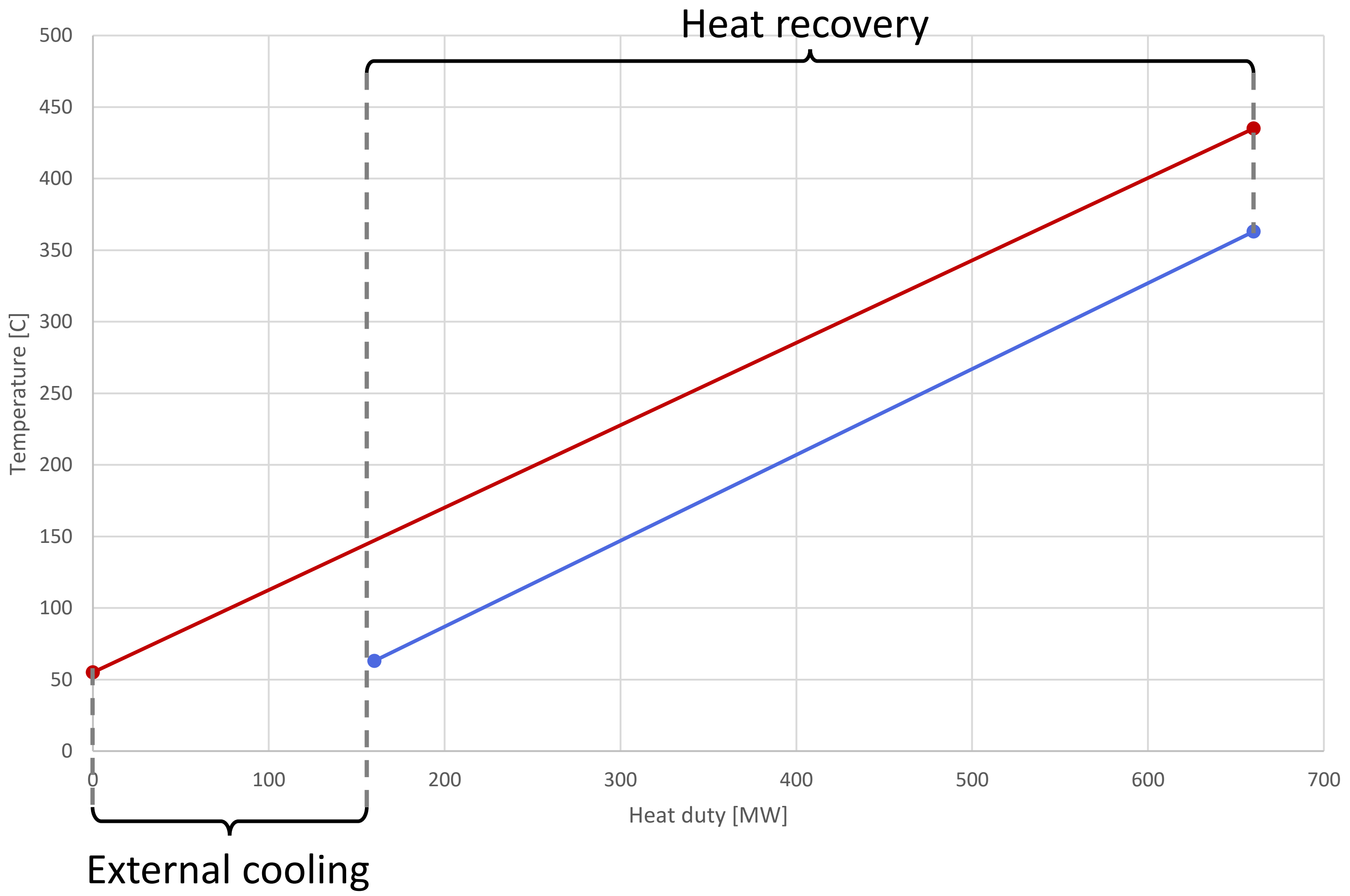
Part 2 – Optimization

Approach

- Heat Recovery with Steam
  - Used low- and high-pressure steam to recover heat from reactor outlet, reducing utility costs.
    - LPS: saturated at 150 °C
    - HPS: saturated at 254 °C
  - Excess steam exported for additional value.
- Reactor Inlet P/T Optimization
  - Case studies showed optimal inlet temperature at 200 bar.
  - Optimized heat exchanger temperatures.
- Feed Compressors
  - Optimized with Electricity consumption as the objective function

Part 2 – Optimization

Approach – Heat Recovery



From
500 MW heating demand and
660 mw cooling demand

To
160 MW cooling demand

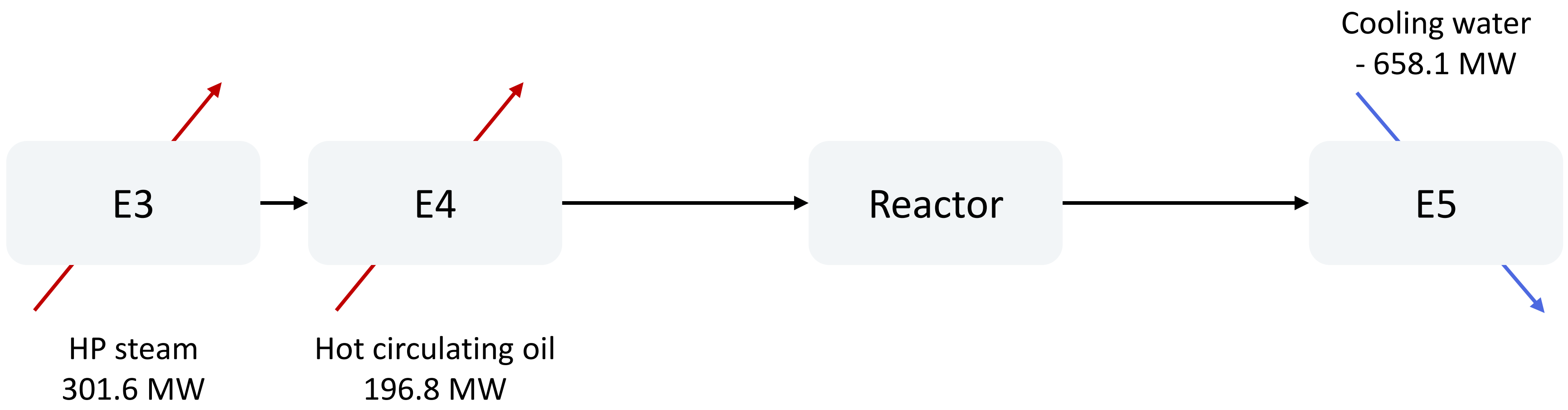
There is enough temperature difference to drive heat exchange

But not as simple as that.. why?

a. Gas - Gas U = 100 W/m2/K
b. Gas - Liquid U = 200 W/m2/K
c. Liquid-Liquid U = 500 W/m2/K
d. Gas - condensing vapor or boiling liquid U = 500 W/m2/K
e. Liquid - condensing Vapor U = 1000 W/m2/K

Part 2 – Optimization

Heat integration – Base case



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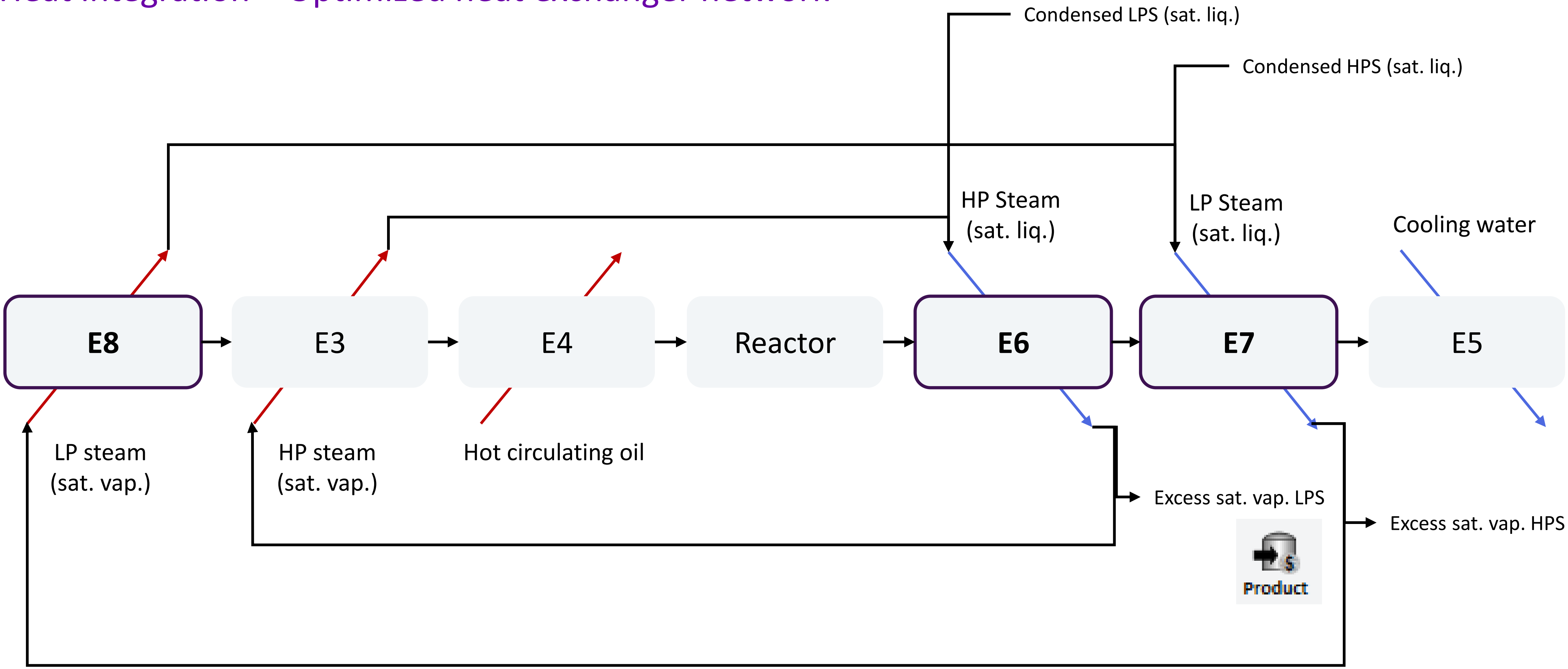
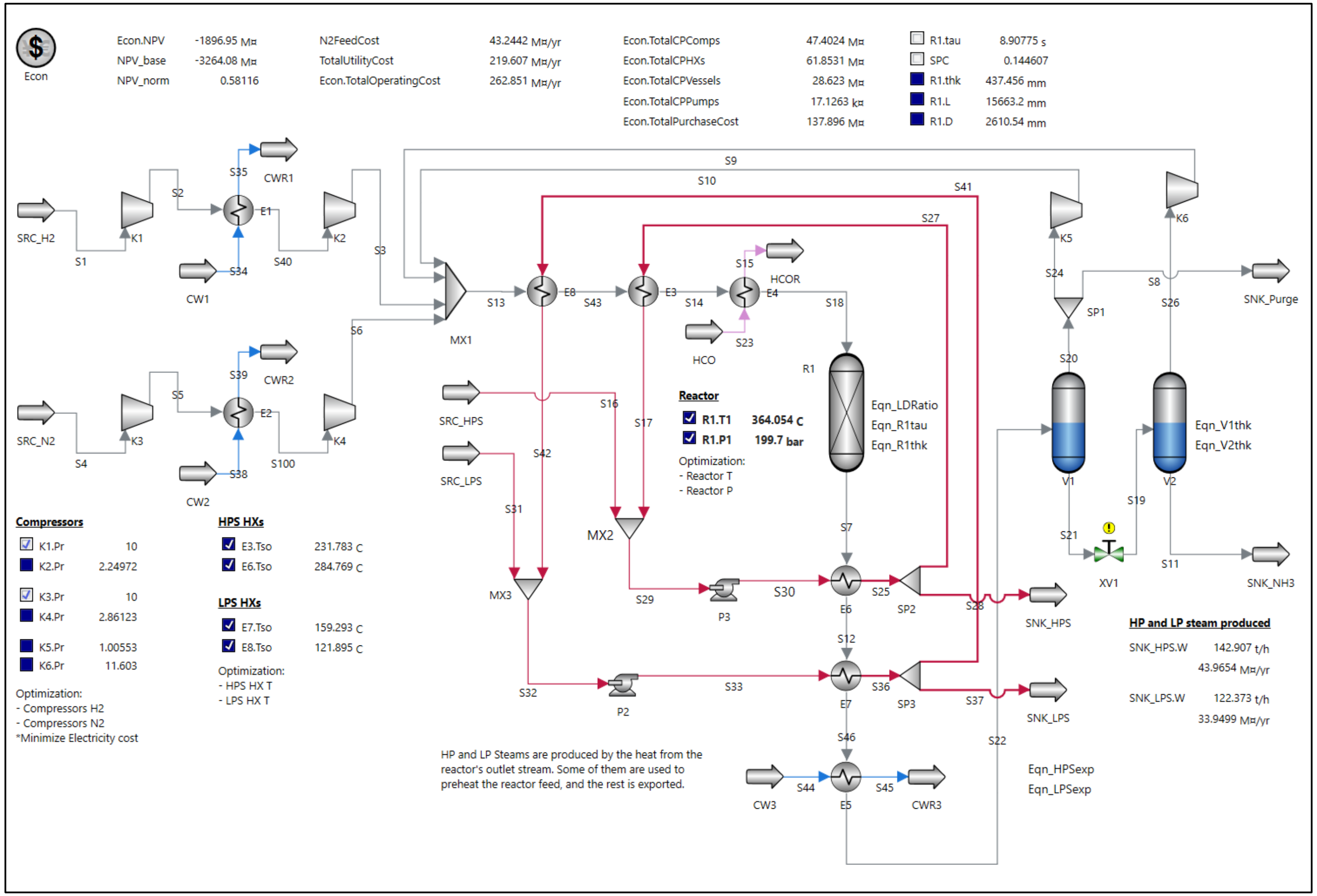
Part 2 – Optimization

Heat integration – Optimized heat exchanger network



Part 2 – Optimization

Flowsheet



Blue: Cooling water

Red: High- and low- pressure steam

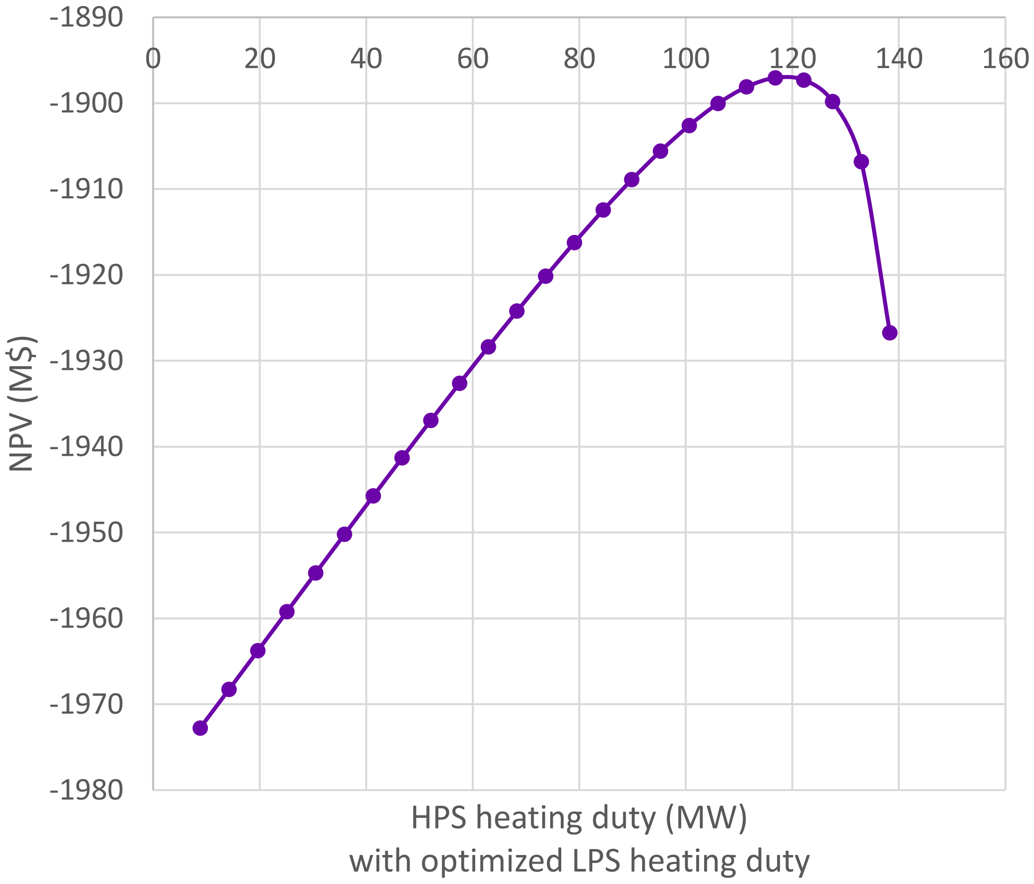
— saturated liquid

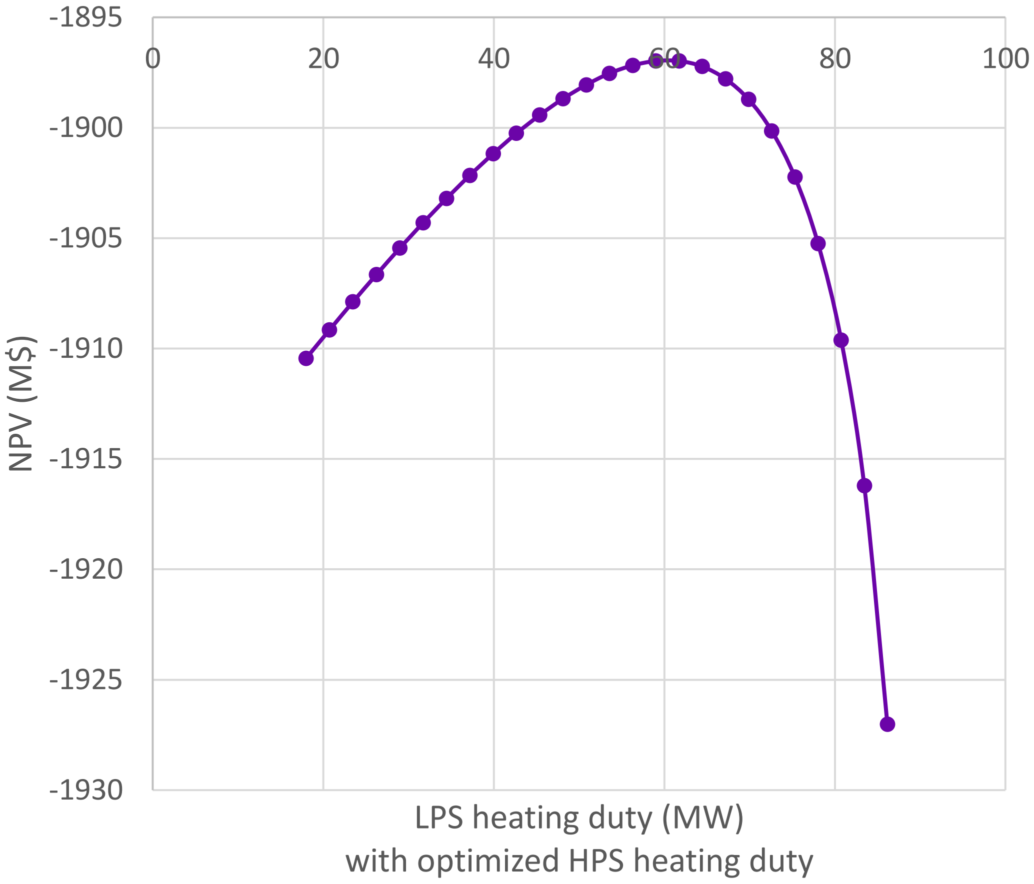
— saturated vapor

Pink: Hot circulating oil

Part 2 – Optimization

Heat exchanger optimization





Part 2 – Optimization

Economic summary

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			

- While the base case **consumes** high-pressure steam (HPS) as a heating medium, high- and low-pressure steam are **net produced** in the optimized process.
- (Net utility cost) = (Total utility cost) – (Product value of exported steam)
- Cost of the feed nitrogen was not considered.
- Steam products that only exist in the optimized process are denoted with an asterisk (*).

Part 2 – Optimization

Economic summary

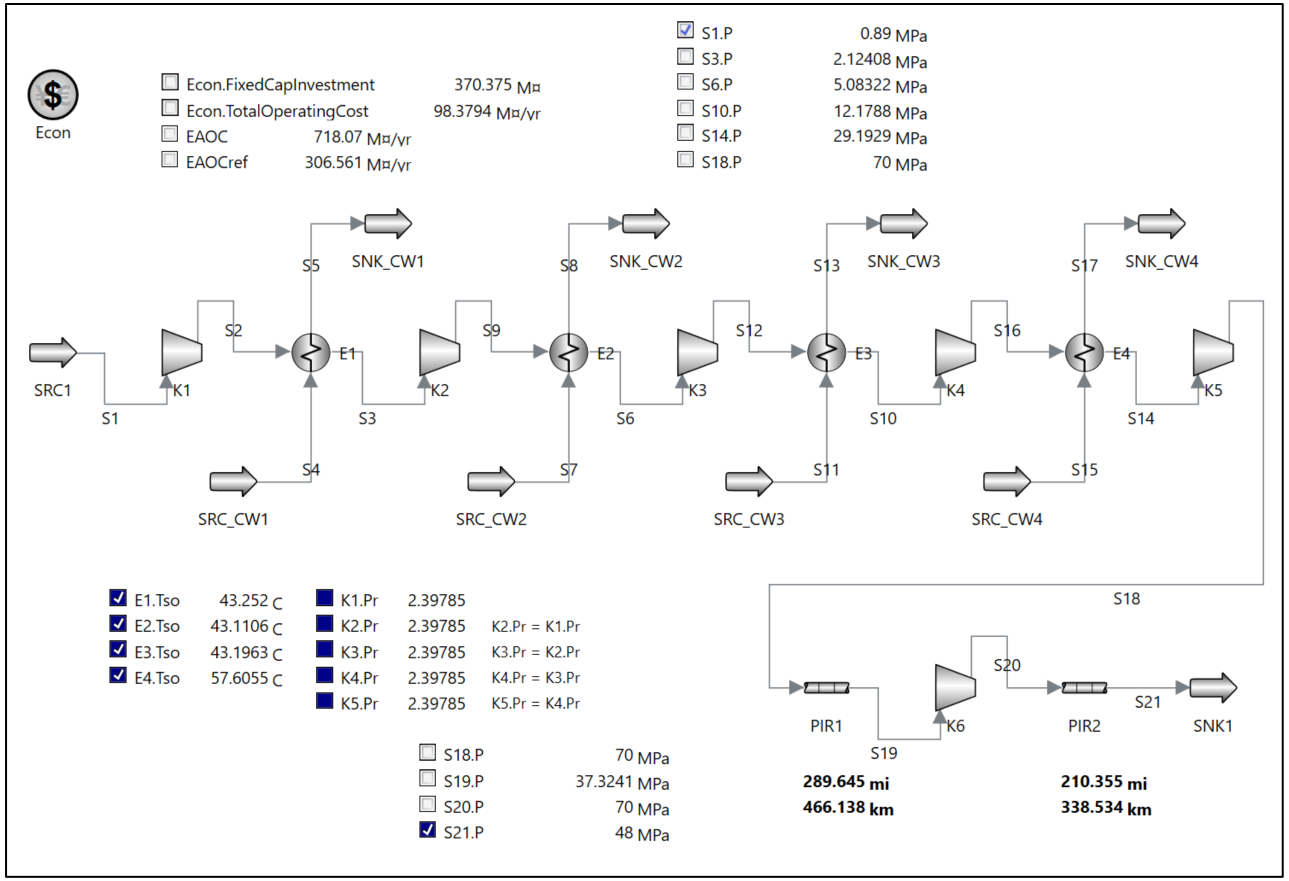
Table 3. Economic summary: Equipment purchase cost.

	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

- Equipment that were added to the base case are denoted with an asterisk (*).

Part 3 – Pipeline design and comparison

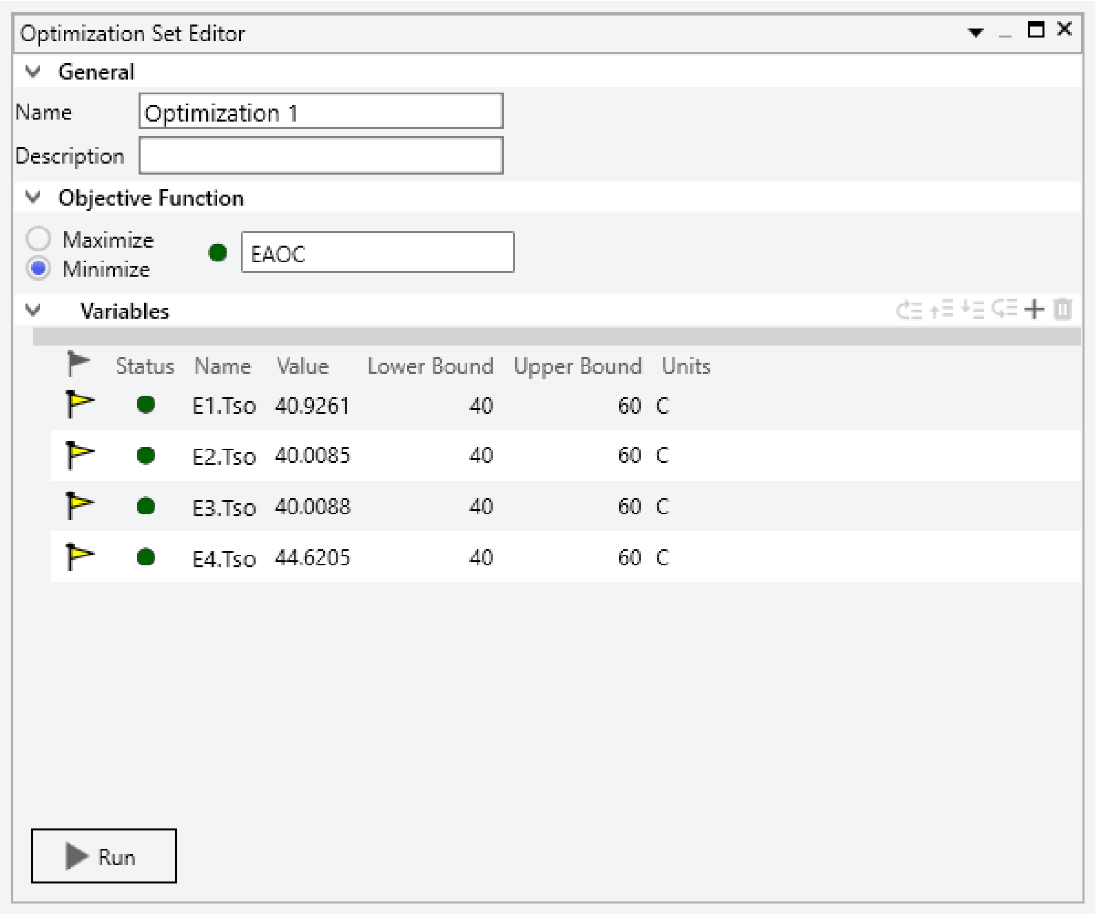
Flowsheet



- "The H_2 should be delivered to the point of use (500 miles from its generation point) at 480 bar."
  - My interpretation: 480 bar at the end of the pipeline.
- H_2 from solar farm at 8.9 bar
- 5-stage compression with compression ratio = 2.4
  - Hydrogen is very hard to compress
- Three main variables:
  - Pipeline 1 pressure drop
  - Pipeline 2 pressure drop
  - Position of the booster station

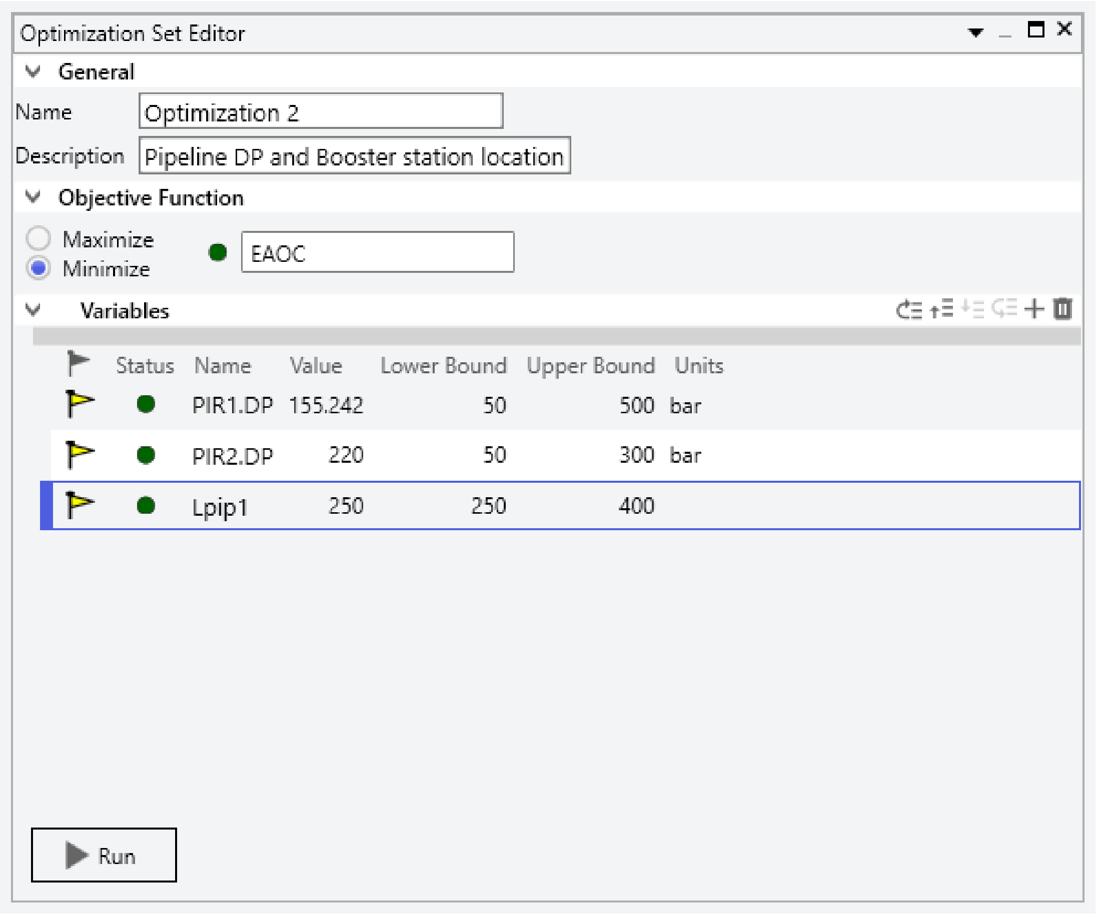
Part 3 – Pipeline design and comparison

Optimization – Intercooler temperatures



Part 3 – Pipeline design and comparison

Optimization – Pipeline pressure drop and booster station location



Part 3 – Pipeline design and comparison

Economic summary and conclusion

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. 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

- Pipeline EAOC = **718.1 M$**
  vs **306.6 M$** (NH3 process)

  $$\text{EAOC [\$/y]} = \text{Total Fixed Capital Investment[\$]}/6\text{ y} + \text{Total Operating Cost [\$/y]}$$

- Using ammonia as a hydrogen carrier is economically a better option than direct transport of pressurized hydrogen.

- There's a catch:
  - Liquid ammonia transport by ships emits CO2
  - Ammonia cracking (or decomposition) to get H2 back
    - Energy intensive
    - Endothermic
    - Requires good catalysts

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Q&A