Supplementary Information

Polygeneration process design to recover waste cold energy in LNG regasification terminals: Simulation-based optimization approach

Hrithika Ganta, Arnab Dutta*

Chemical Engineering Department

Birla Institute of Technology and Science (BITS) Pilani, Hyderabad Campus

Jawahar Nagar, Medchal District, Hyderabad-500078, Telangana, India

Table S1: Critical properties of working fluids.

Working Fluids	Normal Boiling Points (°C)	Critical Temperature (°C)	Critical Pressure (kPa)
Ethane	-88.59	32.28	4883.85
Propane	-42.101	96.75	4256.66
Propylene	-47.75	91.85	4620.41
R23	-82.15	26.15	4860
n-Butane	-0.50	152.05	3796.62
i-Butane	-11.73	134.95	3647.62
R134a	-26.07	101.03	4056
R143a	-47.34	72.73	3764
R152a	-24.99	113.88	4444.44
R125	-48.11	66.02	3619.89
R218	-36.65	71.95	2680
R124	-12.10	122.49	3540
R32	-51.65	78.45	5820
R41	-78.45	41.85	5870

* Corresponding authors: Email: arnabdutta@hyderabad.bits-pilani.ac.in.Tel.: +91 40 66303758.

R161	-37.65	102.15	5019.99
n-Pentane	36.06	196.45	3375.12
i-Pentane	27.87	187.25	3333.59
Methane	-161.52	-82.45	4640.68
R116	-78.25	19.85	3060
R14	-128.04	-45.55	3720
Ethylene	-103.75	9.21	5031.79
R30	39.85	236.85	6070
R245fa	15.30	154.05	3640
R40	-24.05	143.15	6700
R22	-40.75	96.05	4975.04
R13B1	-57.73	66.99	3963.79
R744	-78.46	30.98	7380

Table S2: LNG compositions before HHR process [1].

	Case 1	**Case 2**	**Case 3**
Methane	0.8987	0.8782	0.9226
Ethane	0.0665	0.0830	0.0639
Propane	0.0023	0.0298	0.0091
i-Butane	0.0041	0.0040	0.0021
n-Butane	0.0057	0.0048	0.0022
i-Pentane	0.0001	0.0000	0.0000
Nitrogen	0.0019	0.0001	0.0000

Cost correlations

The capital cost for each equipment is calculated based on its respective size using empirical cost correlations as given in Turton et al [2].

The general equation representing capital cost of an equipment is given as:

Bare module cost: $C_{BM} = C_P * (B_1 + B_2 * F_M * F_P)$

Purchased cost: $C_P = 10\text{^}(K_1 + K_2 * \log_{10} A + K_3 * (\log_{10} A)^2$

Pressure factor: $F_P = 10\text{^}(C_1 + C_2 * \log_{10} P + C_3 * (\log_{10} P)^2$

Material factor: F_M

Bare module factor: B_1, B_2

A = Capacity parameter $[A_{Min} \leq A \leq A_{Max}]$

P = Pressure (barg)

Table S3: Coefficients for evaluating capital cost of different equipment

Coefficients	Heat exchanger [Shell & Tube]	Pump [Centrifugal]	Turbine [Axial gas]
K_1	4.3247	3.3892	2.7051
K_2	-0.3030	0.0536	1.4398
K_3	0.1634	0.1538	-0.1776
C_1	0.03881	-0.3935	---
C_2	-0.11272	0.3957	---
C_3	0.08183	-0.00226	---
F_M	3.2	SS: 2.3	6.1

		Ni: 4.4	
B_1	1.63	1.89	---
B_2	1.66	1.35	---
Capacity parameter	Area (m^2) [10 - 1000]	Power (kW) [1 - 300]	Power (kW) [100 – 4000]
Max. pressure (P_{Max} barg)	140	100	---

Material of construction: LNG/Hydrocarbons: Stainless Steel (SS). Seawater: Nickel (Ni)

The area of heat exchanger is calculated using the following equation:

$$\mathrm{Area} = \frac{\mathrm{Heat\ Load}}{(\mathrm{U} * \mathrm{LMTD})}$$

$\mathrm{LMTD} = \mathrm{Log\ mean\ temperature\ difference}$

$\mathrm{U} = \mathrm{Overall\ heat\ transfer\ coefficient}$

$\mathrm{U} = 1/\left((d_i/d_o) * 1/h_i + 1/h_o + (d_i/d_o) * f_i + f_o + x_w/k_w\right)$

1.5-inch O.D. tube 18 BWG: $d_i = 1.4\ \mathrm{inch}$ $d_o = 1.5\ \mathrm{inch}$ $d_i/d_o = 0.933$

Tube wall resistance: x_w/k_w

$x_w = \mathrm{Wall\ thickness} = 0.049\ \mathrm{inch}$

$k_w = \mathrm{Thermal\ conductivity}_{\mathrm{Stainless\ steel}} = 12\ \mathrm{W/mK}$

$x_w/k_w = 3.403 * 10^{-4}\ \mathrm{m^2K/W}$

Fouling resistance (Shell side: f_o & Tube side: f_i):

$f_{\mathrm{Hydrocarbons}} = 1 * 10^{-4}\ \mathrm{m^2K/W}$

$f_{Seawater} = 2 * 10^{-4}\, m^2K/W$

The values of individual heat transfer coefficients (Shell side: h_o & Tube side: h_i) are obtained from Kreith [3].

Shell: Water ($h = 6250\, W/m^2K$)

Tube: Hydrocarbons vaporizing ($h = 1875\, W/m^2K$)

Shell: Hydrocarbons vaporizing ($h = 1875\, W/m^2K$)

Tube: Hydrocarbons condensing ($h = 1750\, W/m^2K$)

The capital cost of the multi-stream heat exchanger (MSHE) utilized in this study is assessed following the methodology outlined in the literature [4], which offers a graphical representation correlating cost per unit volume (£/m³) to volume (m³). The data from this graph is employed to fit the following power-law equations, enabling the determination of the cost per cubic meter of the MSHE as a function of its volume:

$$\frac{cost}{m^3} = \begin{cases} PF \times 24965 \times volume^{-0.872}, & volume < 0.1 \\ PF \times 45082 \times volume^{-0.645}, & volume < 1 \\ PF \times 45598 \times volume^{-0.535}, & volume \geq 1 \end{cases}$$

Volume range: [0.01-10] m^3, Max. Pressure = 100 bar

$$PF: Pressure\ Factor\ (pressure\ in\ bar) = \begin{cases} 1.00, & Pressure < 25 \\ 1.10, & Pressure < 40 \\ 1.15, & Pressure < 60 \\ 1.25, & Pressure < 80 \\ 1.50, & Pressure \geq 80 \end{cases}$$

The total capital cost (CAPEX) of the process is calculated using the following equation:

$$CAPEX = 1.18 * \left(\sum_{e=1}^{E} C_{BM,e}\right) * {}^{CEPCI_{2024}}/_{CEPCI_{Base}}$$

$\text{CEPCI} = \text{ Chemical Engineering Plant Cost Index}$

$\text{CEPCI}_{2024} = 798.8$

$\text{CEPCI}_{\text{Base}} = 397$ [Base Year: 2001]

$DEP_i = dp_i \times CAPEX \ (i = 1,2,..,6)$

$OPEX = 0.18 \times CAPEX + 1.23 \ \times Raw\ material_{Cost} + Utility_{Cost}$

In this study, the polygeneration process does not involve any external utility and no raw material cost is considered as the working fluid is recycled in a closed loop.

Costing methodology

As depicted in Table S3, specific limitations exist for the capacity parameter applicable to each piece of equipment, defining the range wherein the cost equation remains valid. Therefore, it is preferred to use these correlations within the range specified for each piece of equipment. The methodology utilized for costing in this investigation is depicted in Figure S1.

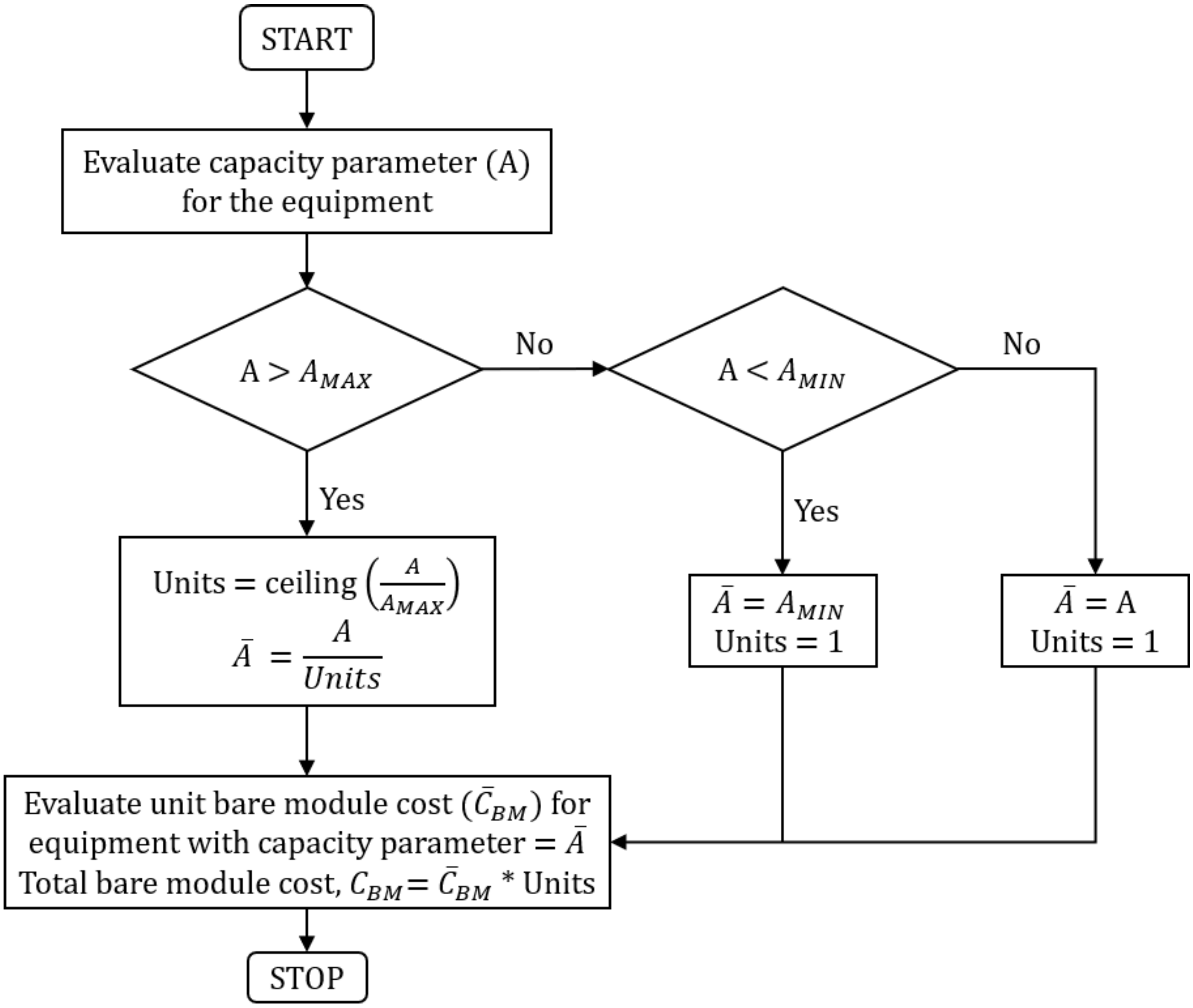

Figure S1: Costing methodology used to calculate bare module cost for each equipment.

References:

1. A. Dutta, I. A. Karimi, and S. Farooq, "Heating Value Reduction of LNG (Liquefied Natural Gas) by Recovering Heavy Hydrocarbons: Technoeconomic Analyses Using Simulation-Based Optimization," *Ind Eng Chem Res*, vol. 57, no. 17, pp. 5924–5932, May 2018, doi: 10.1021/acs.iecr.7b04311.
2. R. Turton, R. C. Bailie, W. B. Whiting, J. A. Shaeiwitz, and D. Bhattacharyya, "Analysis, Synthesis, and Design of Chemical Processes Fourth Edition," 2012.
3. Frank Kreith, *The CRC handbook of thermal engineering*. CRC Press LLC, 2000.
4. G.F. Hewitt, S.J. Pugh, Approximate Design and Costing Methods for Heat Exchangers, Heat Transfer Engineering 28 (2007) 76–86. https://doi.org/10.1080/01457630601023229.