# Energy Network and Portfolio Optimization

# Capstone Project (CP-302)

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# Introduction

The prosperity of modern society depends on the stability of its energy supply. Energy network optimization is a field of study that focuses on optimizing the operation and management of energy systems, including electricity grids, gas pipelines, district heating systems, and other interconnected networks. Energy network optimization focuses on optimizing the operation and management of energy systems, such as electricity grids, gas pipelines, or district heating systems. It involves determining the most efficient and cost-effective way to generate, transmit, distribute, and consume energy within the network. The objective is to ensure reliable and affordable energy supply while considering factors such as generation capacities, transmission constraints, demand patterns, and environmental considerations.

Energy Network optimization when combined with other optimization processes such as Portfolio optimization (PO) facilitates the efficient and sustainable management of energy systems while optimizing financial performance. PO helps to: Identify the optimal mix of energy assets, optimize investment & resource allocation, Incorporate financial & economic considerations.

For example, the electricity distribution network topology of the renewable energy community in Carinthia (in Austria) can be seen in the Figure 1.

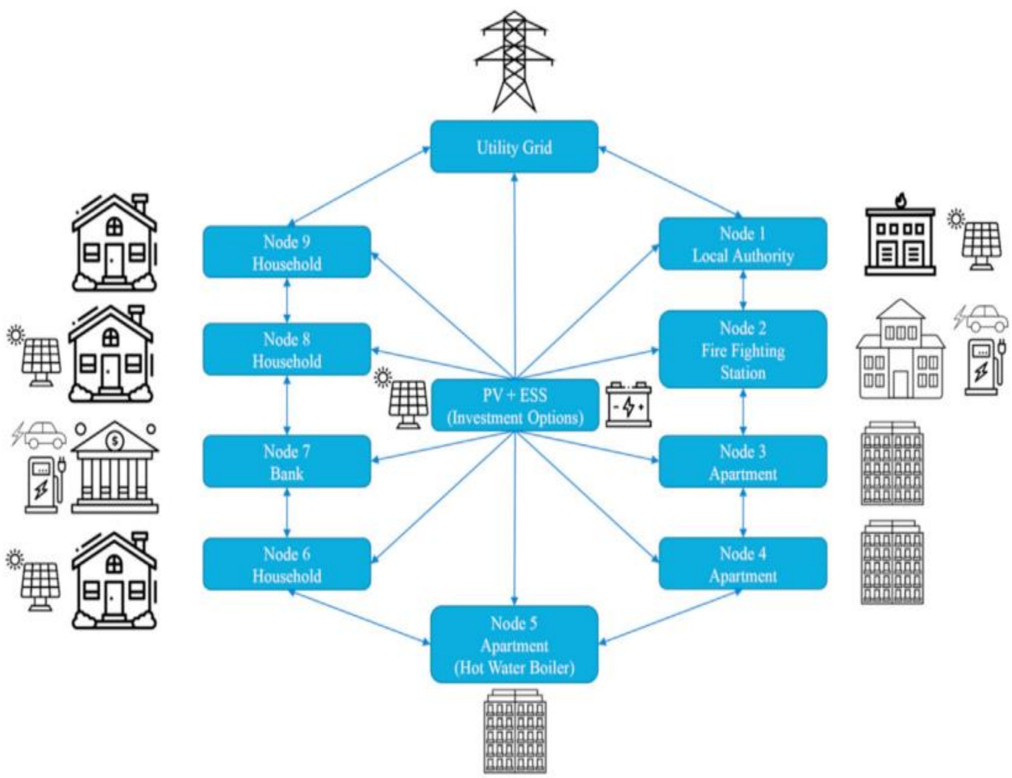


*Figure 1: The network topology of the REC testbed at a village in Carinthia (Austria) with central investment options and other existing technologies.*
*(PV = Photo-Voltaic, ESS = Energy Storage System) (Reference: 1, Pg. no. 6)*

On applying both the Energy network and Portfolio optimization on this network topology, following problem statements can be solved:

1. Do local and renewable energy communities have potential for efficient use of distributed energy technologies at regional levels? (Energy distribution Optimization)
   Decision variables to be considered depend on the number and type of community participants and distributed technologies.

2. Will the expansion of the portfolio of power generation technologies by adding renewable energy bring about an increase in efficiency and reduce risk? (Portfolio optimization)
   Insufficient investment in the electricity sector creates bottlenecks in energy flow.

To solve this problem, following steps can be followed:

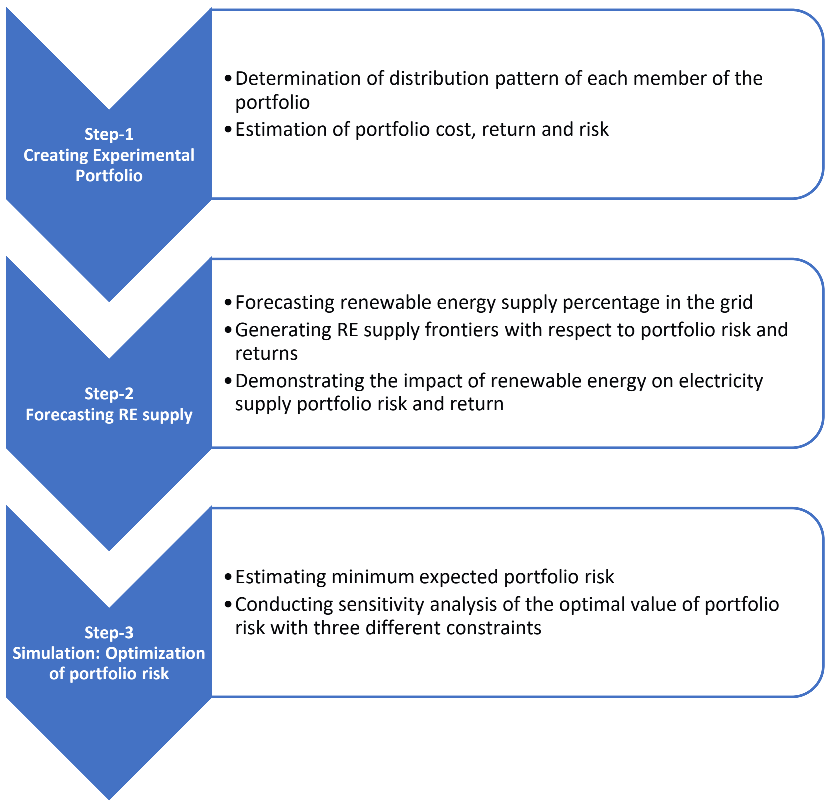


*Figure 2: Steps for Optimization of Renewable Energy Distribution.*
*(Reference: 2, Pg. no. 6)*

For solving this problem, there are various factors considered including, renewable energy generation, power plant capacities, energy demand, storage systems, grid constraints, power plant, fuel costs, emissions, electricity demand projections and much more.

Since, this case study is very complex and involves a large number of concepts to be integrated together, so this report focus on the optimization of the Gas compression system and the methods can be used later in other cases of optimization.

# Introduction to Gas Compression system

A gas compression system is a mechanical system designed to increase the pressure of a gas. Gas compression systems play a vital role in many industries by enabling the transportation of natural gas through pipelines, increasing the pressure of process gases for chemical reactions, storing compressed air for industrial applications, and more. The specific design and configuration of a gas compression system depend on factors such as the type of gas, required pressure levels, flow rates, and environmental conditions.

The design and optimization of gas compression systems plays a critical role in ensuring the efficient and cost-effective transportation of natural gas through pipelines. A key aspect of this design is the optimization of energy consumption, which has significant economic and environmental implications. Thus, there is an increasing need to optimize energy usage while maintaining system performance.

A gas-gathering and transmission system consists of various components such as gas sources, pipeline segments, compressor stations, and delivery sites. Designing or expanding such a system involves considering capital expenditures, operational costs, and maintenance expenses. Numerous factors must be taken into account, including:

1. Determination of the maximum number of compressor stations required within a specified timeframe.
2. Identifying the optimal locations for these compressor stations.
3. Establishing the initial construction dates for the stations.
4. Finding the optimal expansion solutions for the compressor stations.
5. Determining the optimal diameter sizes for the main pipes in each network segment.
6. Considering the minimum recommended thickness of the main pipes.
7. Evaluating the optimal diameter sizes, thicknesses, and lengths of any required parallel pipe loops along each network segment.
8. Planning the timing of construction for the parallel pipe loops.
9. Setting the operating pressures for the compressors and the gas within the pipelines.

This report focuses on a simplified problem of minimizing energy consumption in a gas compression system and explores a few approaches to address this challenge. Network optimization techniques like Linear programming, non-linear programming, Minimum cost flow have been used to model and solve the problem. The objective is to minimize energy usage while ensuring the required gas flow rates and pressures.

Additionally, factors such as pipeline length and diameter changes, which significantly influence the optimal design of gas compression systems have been examined. The insights gained from this analysis will provide valuable guidance to engineers and operators involved in the design and operation of gas compression systems.

## Problem Statement

Here, a system of three compressors operating in series is considered to compress natural gas (practically methane) from an initial pressure $P_0$ to a desired pressure $P_f$ (see Fig. 1). After the first and the second compressor, there is an intercooler located with the aim to lower the temperature to the initial temperature $T_0$.

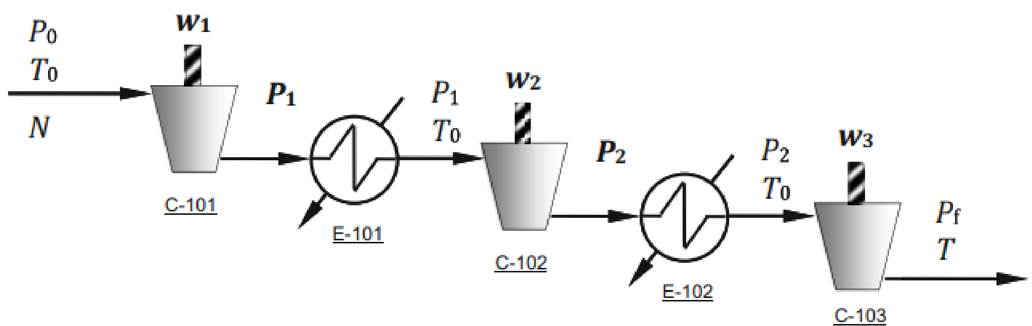


*Figure 3: Three compressor System*
*(Reference:4, Pg. no. 74)*

The power W consumed by a compressor to compress a gas from initial pressure $P_{in}$ and absolute temperature $T_{in}$ to a final pressure Pout is determined in undergraduate thermodynamics books and is given by:

$$W = N * \frac{1}{e} * \frac{RT_{in}}{a} * \left[ \left( \frac{P_{out}}{P_{in}} \right)^{a} - 1 \right]; \quad a = \frac{C_p / C_v - 1}{C_p / C_v} > 0$$

*Equation 1*

where N is the molar flow rate of the gas, R is the ideal gas constant, e (<1) is the fractional efficiency with respect to a reversible adiabatic compression, and $C_p$ ($C_v$) is the constant pressure (volume) heat capacity.

As the temperature in the suction of all the compressors is the same, the function for total power consumed for the three-compressor system can be gives as:

$$f(P_1, P_2) = \frac{W_1 + W_2 + W_3}{N \frac{1}{e} \frac{RT_{in}}{a}} = \left( \frac{P_1}{P_0} \right)^{a} + \left( \frac{P_2}{P_1} \right)^{a} + \left( \frac{P_f}{P_2} \right)^{a} - 3$$

*Equation 2*

where W1, W2 and W3 is the energy consumed by compressor 1, 2 and 3 respectively. $P_0$, $P_1$, $P_2$, and $P_f$ (or $P_3$) are the respective pressures as shown in Figure 1.

Note that the expression f ($P_1$, $P_2$) is unitless and does not directly represent the total power consumption of the three-compressor system. Hence, the total power consumption of the three-compressor system will be given by the following expression:

$$W_{Total} = W_1 + W_2 + W_3 = \left( \mathrm{N} * \frac{1}{e} * \frac{\mathrm{RT_{in}}}{a} \right) * f\ (P_1, P_2)$$

*Equation 3*

# Approaches:

Below mentioned are the four approaches to solve this problem statement. The **first** approach is the "Theoretical Method" approach, according to which, the objective function is defined, and the possibility of a minimum is investigated by calculating the first derivative. The exact values of the intermediate pressures are determined, and the total energy consumed is calculated based on the obtained pressures. In the **second** approach, The MATLAB code implementing Newton's method is described, which takes the objective function, gradient, Hessian, and initial guess as inputs. The function implementing the Newton's method needs to be defined. The code iteratively refines the guess until it converges to a minimum. In the **third** approach, the "fminunc" function in MATLAB is introduced as a command for unconstrained optimization. The function itself finds a local minimum of a function of several variables, without requiring the gradient, hessian matrix and newton's method function to be defined. In the **fourth** approach, the MATLAB code is written to create "3D and 2D contour plots" of the objective function as a function of the two variables. The code evaluates the objective function at each point on the grid and plots the function using the surf and contour functions. Both plots help to visualize the location of the minimum point of the curve, at which the of P1, P2, and the objective function values are obtained.

NOTE: For all the approaches, the 3 compression stages increase the pressure from 1 to 10 bar, i.e., $P_0$ = 1 bar and $P_f$ = 10 bar. Also, for calculating the total power consumption the other values are taken as; N=60 moles/second, e=0.75, $T_{in}$= 320 K, R = 8.314 J/mol-K, a= 0.3.

## 1. Theoretical Method

The objective function of the problem is:

$$\mathrm{f}\ (\mathrm{P_1}, \mathrm{P_2}) = \left(\frac{\mathrm{P_1}}{P_0}\right)^{\mathrm{a}} + \left(\frac{\mathrm{P_2}}{P_1}\right)^{\mathrm{a}} + \left(\frac{\mathrm{P_f}}{P_2}\right)^{\mathrm{a}} - 3$$

*Equation 4*

This is a function of two variables, $P_1$ and $P_2$. To investigate the possibility of a minimum to exist, the first derivative with respect to $P_1$ and $P_2$ is calculated as:

$$\nabla f_{P_2}^{P_1} = \begin{matrix} a\,\dfrac{1}{P_1}\left[\left(\dfrac{P_1}{P_0}\right)^a - \left(\dfrac{P_2}{P_1}\right)^a\right] \\ a\,\dfrac{1}{P_2}\left[\left(\dfrac{P_2}{P_1}\right)^a - \left(\dfrac{P_f}{P_2}\right)^a\right] \end{matrix}$$

*Equation 5*

Now, by setting the gradient equal to zero, the following result is obtained:

$$\frac{P_1}{P_0} = \frac{P_2}{P_1} = \frac{P_f}{P_2} = \lambda$$

*Equation 6*

Please note that the ratio of the delivery to suction pressure (known as compression ratio λ) for the 3 compressors is equal, i.e., at the optimal point, the compression ratios of the three compressors are equal.

To determine the exact value of the intermediate pressures, the following calculation is done:

$$P_f = \lambda\, \mathrm{P}_2 = \lambda^2 P_1 = \lambda^3 P_0$$

*Equation 7*

$$or$$

$$\lambda = \sqrt[3]{\frac{P_f}{P_0}} = \sqrt[3]{\frac{10}{1}} = 2.15443469$$

and therefore, the pressures are $P_1$ = 2.15443469 bar and $P_2$ = 4.641588834.

$$\mathrm{W} = \mathrm{N}\,\frac{1}{e}\,\frac{\mathrm{RT_{in}}}{a}\left[\left(\frac{\mathrm{P_1}}{P_0}\right)^{\mathrm{a}} + \left(\frac{\mathrm{P_2}}{P_1}\right)^{\mathrm{a}} + \left(\frac{\mathrm{P_f}}{P_2}\right)^{\mathrm{a}} - 3\right]$$

*Equation 8*

Total Energy Consumed, $W_{Total}$ = 551092.7037 Watts

## 2. MATLAB implementation of Newton's method to solve the problem numerically.

The Newton method, also known as the Newton-Raphson method, is a popular optimization algorithm used to find the minimum (or maximum) of a function by finding the roots of the derivative (or gradient) of the function and iteratively updating the search direction to approach the minimum.

At each iteration, the method calculates the second-order derivative (or Hessian) of the function and uses it to compute the search direction. The algorithm then updates the current point by taking a step in the direction of the minimum of the quadratic approximation of the function at the current point.

MATLAB code for this can be see in Appendix-A. The defined **myNewton** function in the code takes in the function, gradient, Hessian, and initial guess, and iteratively refines the guess until it converges to a minimum. Once the root is found, the final variable values are stored in **x** and gives the objective function value. Additionally, the code calculates the total energy consumed based on the obtained root and other specified parameters.

```
>> Newton_Implementation
P1 (bar) = 2.1544
P2 (bar) = 4.6416
Objective function value = 0.77678
Total Energy Consumed (Watts) = 551092.7037
```

*Figure 4: Output of MATLAB Implementation of Newton's Method*

## 3. MATLAB Implementation using 'fminunc' function.

This approach considers the command available in MATLAB for unconstrained optimization:

$X_{opt}$ = fminunc (fun, $x_0$, options)

This function finds a local minimum of a function of several variables. Starts at $x_0$ and attempts to find a local minimizer $X_{opt}$ of the function fun. fun (an inline function or an m-file) returns the value of the objective function. It may also return the gradient in which case one must use [f,g]=fun(x) and: options=optimoptions ('fminunc', 'SpecifyObjectiveGradient', true). Also, 'Diplay', Iter is used to display intermediate results.

A distinct advantage of the MATLAB implementation is that it does not require the hessian or the gradient as it builds them numerically. To solve the gas compression problem, the problem description along with the objective function to the fminunc function has been provided, which iterates as per the conditions mentioned in options function and then takes the initial guesses for the two unknown variables (MATLAB code in Appendix-B). The fminunc function accepts the two intermediate pressures as inputs and returns the value of the objective function after a number of iterations as:

```
>> fminunc_Implementation
                                                        First-order
 Iteration  Func-count       f(x)        Step-size       optimality
     0           3         0.778671                        0.00639
     1           9         0.778294             10          0.0054
     2          12         0.776876              1         0.00289
     3          15         0.776777              1         0.00021
     4          18         0.776776              1        1.01e-05
     5          21         0.776776              1         1.4e-06
     6          24         0.776776              1        1.28e-08

Computing finite-difference Hessian using objective function.

Local minimum found.

Optimization completed because the size of the gradient is less than
the value of the optimality tolerance.

<stopping criteria details>
P1 (bar) = 2.1544
P2 (bar) = 4.6416
Minimum Energy function value= 0.77678
Total Energy Consumed (Watts) = 551092.7037
```

*Figure 5: Output of MATLAB Implementation using 'fminunc' function*

## 4. Graphical Method

In this method, a MATLAB code creates a 3D and 2D contour plot of a function f as a function of two variables $P_1$ and $P_2$ (MATLAB code in Appendix-C)

The values of $P_1$ and $P_2$ are generated using the linspace function, which creates an array of evenly spaced values between the minimum (=1) and maximum (=10) values specified.

Next, the meshgrid function is used to create a grid of points from the $P_1$ and $P_2$ arrays, which are used to evaluate the function f at each point on the grid. The for loop iterates over each value of $P_1$ and $P_2$ and calculates the corresponding value of f using the equation provided.

The resulting values of f are stored in the f array, which is then plotted using the surf function to create a 3D surface plot of f as a function of $P_1$ and $P_2$. This plot shows the overall shape of the function and helps to visualize the location of the minimum point.

Finally, the contour function is used to create a 2D contour plot of f as a function of $P_1$ and $P_2$, which shows the contours of constant f values on a 2D plane. This plot can be used to determine the location of the minimum point and to visualize the behavior of the function in more detail.

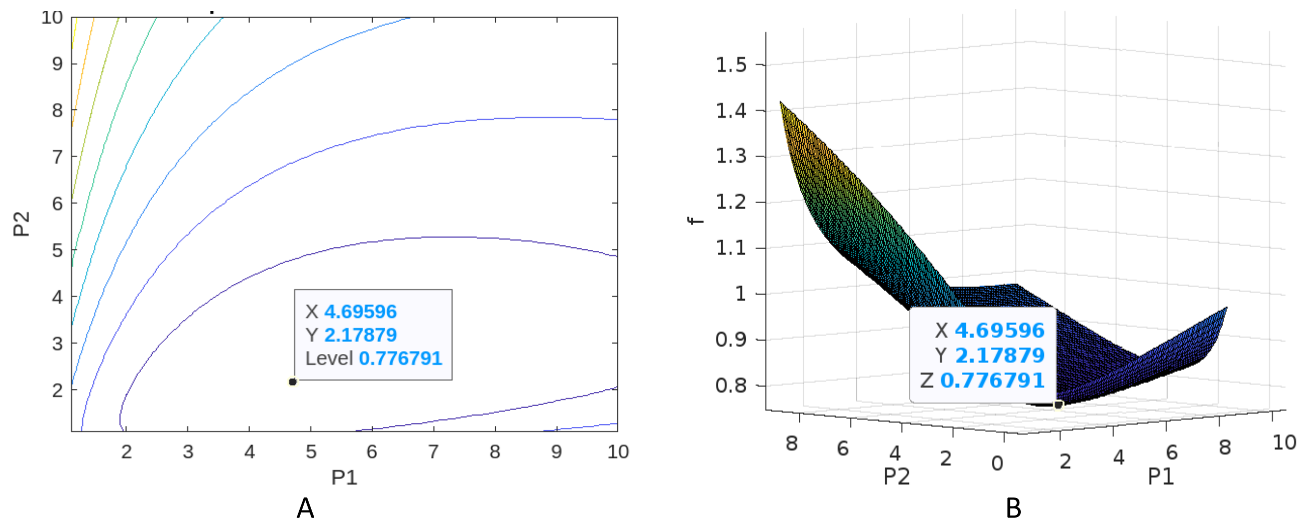


*Figure 6: A) Contour plot of f as a function of $P_1$& $P_2$; B) Surface plot of f as a function of $P_1$& $P_2$*

Here, $P_1$ = 4.69596 bar, $P_2$ = 2.17879 bar, and f ($P_1$, $P_2$) = 0.776791, at the minimum or the most optimal point.

Hence, from this method; $W_{Total}$ = 684083.3712 Watts

## Results and Discussion

Among the four approaches above, the first three approaches have given exactly the same optimal values for the pressures $P_1$ and $P_2$ at the given conditions, but in approach 4, the values of $P_1$ and $P_2$ are different from the other three approaches making the f ($P_1$, $P_2$) function value 0.001% greater and making the $W_{Total}$ value 24.13% greater than the values that we got from the other three approaches.

In each approach, there are some major limitations which are mentioned below:

1. In approach 1, we have calculated the gradient and the hessian of the objective function w.r.t to 2 variables, making this approach very difficult to follow when there are more number of variables.
2. In approach 2, we have not only calculated the gradient and the hessian of the objective function but also had to write the code for defining the Newton's method. Although, it reduced our calculation, but still, it would be very hard to follow this approach when there will be more variables.
3. Approach 3 is the most preferred method as it not only consumes less effort to solve the problem, but also gives accurate answers. But this method will also fail when we will

required to solve linear and non-linear functions with certain equality and inequality constraints. In that case, we prefer to solve the problem with the "fmincon" function.

4. Approach 4 gives the good visual idea about the number and type of extremum value, which could help us to narrow down the range of the most optimal value, but it is the least dependent method for finding the exact optimal value of variables and objective function. It not only give the wrong value but also makes it hard to pin-point the exact minimum or maximum value with the increasing complexity of the graph.

The Newton method can converge to the minimum very quickly, especially for well-behaved convex functions, and can be more efficient than other optimization algorithms. However, the method can be computationally expensive, especially for functions with large Hessian matrices, and may not converge if the Hessian is not positive-definite.

In practical scenarios, gas compressors systems are much more complex with large number of branches of pipeline to be integrated in order to meet the specific demands at different locations and at different times. In those scenarios, we also prioritize the operation of the whole system to be economically sustainable and has to deal with large number of constraints (demographic, geographic, operational, market related, quality targets, political, consumption, etc.), without compromising with the efficiency and quality of the process. In such pipeline networks, to solve the operational problems, we follow non-linear optimization, Mixed Integer Linear programming and the branch & bound type of approaches to find the required variable values. Obviously, a high simulation power is also required to process such heavy simulations.

A multi-branched pipeline network of compressors can be considered as a complex geometry diagram which further connects to several other systems to meet the supply and demand equilibrium. This involves aggregation of demand from different systems to their nearest pipeline. It starts by buffering the complex geometry to enlarge it be a given length in all directions. This property is shown in the skeletonization algorithm below to generalize densely connected street segments.

## Verification with DWSIM Simulation

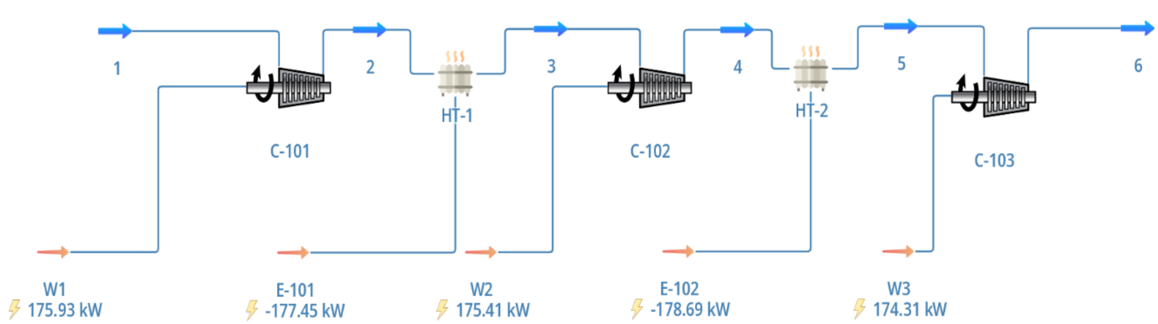


*Figure 7: DWSIM-SIMULATION*

A three-compressor system in the DWSIM is made (see Figure 5) to verify if the calculated total power consumed in the process through different approaches is matching the total power consumed in the DWSIM simulation or not, keeping the same inputs and operating conditions. Through DWSIM simulation, the values of heat energy supplied by the Heater to maintain the constant temperature throughout the process can also be obtained (since, temperature is reduced using the Heater, so we got the negative values of the heat supplied).

So, from the simulation the total power consumed by the three compressors can be calculated to be: $W_1 + W_2 + W_3$ = (175.93 + 175.41 + 174.31) KW = 526.65 KW, which is very close to the total power consumed value calculated through our approaches i.e., 551 KW. The error is around 4.623% only.

Also, Total Heat energy supplied by the Heater to maintain the constant temperature can be calculated to be: $E_{101} + E_{102}$ = -(177.45+178.69) KW = - 356.14 KW.

Hence, the total power requirement to operate this system for the desired results can be calculated as: $(W_1 + W_2 + W_3) – (E_{101} + E_{102})$ = 526.65 KW + 356.14 KW = 882.79 KW.

The respective DWSIM simulation file and the Properties Table Data of the system can be accessed through the links provided in Appendix-D

## Case Study

The task is to optimize the design of a pipeline system to transport natural gas from an initial pressure, $P_0$ (= 300 psi) to a final point $P_f$ (= 400 psi). The system consists of four-compressors, and they all are connected with the help of three pipeline segments. The goal is to minimize the following cost function (dollars per year) associated with the design while satisfying certain constraints.

$$f = \sum_{i=1}^{n} (C_0 + C_c) * Q * (0.08531) * T * \left(\frac{k}{k-1}\right) * \left[\left(\frac{P_{d_i}}{P_{s_i}}\right)^{\frac{z*(k-1)}{k}} - 1\right] + \sum_{j=1}^{m} C_s * L_j * D_j$$

*Equation 9*

Where,

- n = number of compressors in the system;
- m = number of pipeline segments in the system (= n + 1);
- $C_0$ = yearly operating cost \$/(hp)(year);
- $C_c$ = compressor capital cost \$/(hp)(year);
- $C_s$ = pipe capital cost \$/(in)(mile)(year);
- $L_j$ = length of pipeline segment j, mile;
- $D_j$ = diameter of pipeline segment j, inches
- k = $C_p/C_v$ for gas at suction conditions
- z = compressibility factor of gas at suction conditions (z ranges from 0.88 to 0.92)
- $P_s$ = suction pressure, psi
- $P_d$ = discharge pressure, psi
- T = suction temperature, °R
- Q = flow rate into the compressor, MMCFD (million cubic feet per day)

<u>Given Values:</u>

- $C_0$ = 14 \$/(hp)(year)
- $C_c$ = 70 \$/(hp)(year)
- $C_s$ = 870 \$/(hp)(year)
- Q = 600 MMCFD (million cubic feet per day)
- T = 520°R
- z = 0.9
- k = 1.26

Assumptions:

- Temperature is constant through out the system i.e., $T_1$
- Length and Diameter of all the pipe segments is the same

Design Variables:

- $P_1$, $P_2$, $P_3$: Pressures at the intermediate points along the pipeline (psi)
- Length, L: Length of each pipeline segment (miles)
- Diameter, D: Diameter of the pipeline (inch)

Constraints:

1. Equality Constraints:
    - Flow Equation: The flow equation must be satisfied at each compressor station.
    - The Weymouth relation (GPSA handbook, 1972), must hold in each pipeline segment:

$$Q = A * D_j^{\frac{8}{3}} * \left[\frac{P_d^2 - P_s^2}{L_j}\right]^{\frac{1}{2}}$$

*Equation 10*

where Q = a fixed number (Flow rate); $P_d$ = the discharge pressure at the entrance of the segment; $P_s$ = the suction pressure at the exit of the segment

To avoid problems in taking square roots, Equation 10 is squared to yield:

$$A^2 * D_j^{\frac{16}{3}} * (P_d^2 - P_s^2) - L_j * Q^2 = 0$$

*Equation 11*

- The flow equation ensures the conservation of mass and energy along the pipeline.

2. Inequality Constraints:
    - Pressure Constraints: The pressure at each point along the pipeline must satisfy a certain condition, i.e., the compression ratio does not exceed some prespecified maximum limit K;

$$\frac{P_{d_i}}{P_{s_i}} \geq K, \qquad i = 1, 2, 3$$

*Equation 12*

- The pressure constraints ensure that the pressure drop along the pipeline remains within acceptable limits.

$$P_0 \leq P_1, P_2, P_3 \leq P_f$$
$$4 \leq L_i \leq 50$$
$$20 \leq D_i \leq 100$$

*Equation 13*

<u>Objective:</u> Minimize the cost function associated with the pipeline system design.

- The cost function comprises operating costs, compressor capital costs, and pipe capital costs.
- The operating cost is influenced by the gas flow rate, temperature, pressure, and physical properties of the gas.

<u>Solution:</u> (MATLAB code in Appendix-E)

- The initial guess for the design variables is assumed as $x_0$.
- Lower bounds (lb) and Upper bounds (ub) are specified for each design variable.
- The optimization is performed using the "fmincon" function with suitable options, because fminunc function does not support applying any constraints in the objective function.
- All the given equality and inequality constraints are applied in the iteration.
- A modified Objective function suitable to do iteration is then defined.
- Following optimized values for the respective variables are obtained:

```
P1 (psi) = 310
P2 (psi) = 348.7493
P3 (psi) = 377.8121
Length (miles) = 24.2188
Diameter (inch) = 35.4199
Minimum Cost function ($/yr): 3157236.953
```

*Figure 8: Case-Study Output values*

The task was to find the optimal values for $P_1$, $P_2$, $P_3$, Length, and Diameter that minimize the cost function while satisfying the given constraints. Here, the cost is coming very may be because we are working in very high-pressure range.

Please note that the above problem can be further modified by not considering the assumptions made, by increasing the number of variables (eg: Q, T, n), by considering branching systems, etc. to make the problem more practical.

## Conclusion

By combining the strengths of energy network optimization and portfolio optimization, stakeholders in the energy sector can make informed decisions regarding energy asset selection, operation, and allocation. In this report, we have addressed the problem of energy network optimization in a gas compression system. The objective was to minimize energy consumption while maintaining the required gas flow rates and pressures. Four approaches were explored: theoretical method, MATLAB implementation of Newton's method, MATLAB implementation using the 'fminunc' function, and graphical method. The resulting pressures were found to be $P_1$ = 2.15443469 bar and $P_2$ = 4.641588834 bar, with a total power consumption of 551092.7037 Watts.

The theoretical method provided an analytical solution by finding the optimal values for the intermediate pressures. The MATLAB implementation of Newton's method involved iteratively refining initial guesses for the pressures until convergence to a minimum. The 'fminunc' function in MATLAB was used for the implementation, which numerically built the gradient and Hessian. The resulting pressures and total power consumption were found to be consistent with the theoretical method. The graphical method visualized the objective function as a 3D surface plot and a 2D contour plot. It provided insights into the behavior of the function and helped determine the location of the minimum point. The obtained pressures and total power consumption from this method were slightly different from the other approaches but still provided valuable information.

Based on the results and discussions, each approach had its limitations and advantages. The results from the approaches was compared with a DWSIM simulation output of the same gas compression system and found the only 4.06% error in the power consumed by three compressors. Through DWSIM simulation helped in calculating the additional heat energy that was needed to keep the temperature value constant.

After that, a case study with more number of variables and a number of equality and inequality constraints was performed to find the optimal minimum value of the objective function for calculating dollars per year expense of the complete system.

In practical scenarios, gas compression systems involve complex networks with numerous variables and constraints. Non-linear optimization, mixed-integer linear programming, and branch and bound methods are commonly employed for solving operational problems in such systems.

Overall, the insights gained from this study will be valuable for engineers and operators involved in the design and operation of gas compression systems. The optimization approaches discussed can be extended and adapted to more complex scenarios, taking into account additional constraints and variables to achieve economically sustainable and efficient energy networks.

# Appendix

## A. Newton_Implementation MATLAB Code

```
clear

a = 0.3;
P0 = 1;
Pf = 10;

f = @(x) (x(1)/P0)^a + (x(2)/x(1))^a + (Pf/x(2))^a - 3;
F = @(x) [(a*((x(1)/P0)^a - (x(2)/x(1))^a))/x(1);
          (a*((x(2)/x(1))^a - (Pf/x(2))^a))/x(2)];
H    =    @(x)    [(a*((x(2)/x(1))^a    -    (x(1)/P0)^a    +    a*(x(1)/P0)^a    +
a*(x(2)/x(1))^a))/x(1)^2, -(a^2*(x(2)/x(1))^a)/(x(1)*x(2));
          (a^2*(x(2)/x(1))^a)/(x(1)*x(2)),  (a*((Pf/x(2))^a  -  (x(2)/x(1))^a  +
a*(x(2)/x(1))^a + a*(Pf/x(2))^a))/x(2)^2];

x = myNewton(f, F, H, [2;4]);

disp(['P1 (bar) = ' num2str(x(1))]);

disp(['P2 (bar) = ' num2str(x(2))]);

disp(['Objective function value = ' num2str(f(x))]);

    N = 60; % moles/second
    e = 0.75;
    Tin = 320; % temperature in K
    R = 8.314; % gas constant
    a = 0.3;

    %W1+W2+W3
    Total_energy = N * (1 / e) * R * (Tin / a) * (f(x));

disp(['Total Energy Consumed (Watts) = ' num2str(Total_power)]);

function x = myNewton(f, F, H, x0)
% MYNEWTON  Find the root of a function using Newton's method.
%    X = MYNEWTON(F, FPRIME, X0) finds the root of the function F using
%    Newton's method, starting at X0.

MAX_ITERS = 100; % Maximum number of iterations
TOL = 1e-6;      % Tolerance for stopping criterion

for k = 1:MAX_ITERS
```

```
    fx = f(x0);
    if norm(fx) < TOL
        break;
    end

    J = F(x0);
    Hx = H(x0);

    % Check if Hessian is positive definite
    [~, p] = chol(Hx);
    if p ~= 0
        warning('Hessian is not positive definite.');
        break;
    end

    dx = -Hx \ J;
    x0 = x0 + dx;
    % To display iteration (all the 100) at every point:
    %fprintf('iter:  %d,  x1:  %.6f,  x2:  %.6f,  f:  %.6f\n',  k,  x0(1),  x0(2),
norm(fx));

end

x = x0;
end
```

## B. Fminunc_Implementation MATLAB Code

```
options=optimoptions('fminunc','Display','iter');
[x,fval]=fminunc(@ThreeStageCompression,[2;4],options);

disp(['P1 (bar) = ' num2str(x(1))]);

disp(['P2 (bar) = ' num2str(x(2))]);

disp(['Minimum Energy function value= ' num2str(fval)]);

    N = 60; % moles/second
    e = 0.75;
    Tin = 320; % temperature in K
    R = 8.314; % gas constant
    a = 0.3;
    %W1+W2+W3
    Total_energy = N * (1 / e) * R * (Tin / a) * (fval);

disp(['Total Energy Consumed (Watts) = ' num2str(Total_energy)]);

function f=ThreeStageCompression(P)

P0 = 1; % initial pressure in bar
Pf = 10; % final pressure in bar
a =0.3; % parameter of the model

f= (P(1)/P0)^a + (P(2)/P(1))^a + (Pf/P(2))^a - 3;
```

```
end
```

## C. Graphical Method MATLAB Code

```
clear all;

P0 = 1; % initial pressure in bar
Pf = 10; % final pressure in bar
a = 0.3; % parameter of the model

P1 = linspace(1.1, 10, 100); % values of P1 between 0.1 to 10
P2 = linspace(1.1, 10, 100); % values of P2 between 0.1 to 10

[f, P] = meshgrid(linspace(-4, 4, 100), linspace(1.1, 10, 100));

for I = 1:length(P1)
    for j = 1:length(P2)
        f(I,j) = (P1(i)/P0)^a + (P2(j)/P1(i))^a + (Pf/P2(j))^a – 3;
    end
end

figure;
surf(P1, P2, f)
xlabel(‘P1’)
ylabel(‘P2’)
zlabel(‘f’)
title(‘Surface plot of f as a function of P1 and P2’)

figure;
contour(P1, P2, f, linspace(-4, 4, 100))
xlabel(‘P1’)
ylabel(‘P2’)
title(‘Contour plot of f as a function of P1 and P2’)
```

## D. DWSIM files

- DWSIM_Simulation_File (.dwxmz)
  https://drive.google.com/file/d/1Hnlo5fk7envKYLjTFZ0jy6HH-dmixYre/view?usp=share_link

- Properties_Table:
  https://docs.google.com/spreadsheets/d/196lHR3Ju9ajqYoRFyEu8ANqpdfpMFr9f4z_X3qIDizM/edit?usp=share_link

## E. Case Study MATLAB Code

```
% Set the initial guess (P1, P2, P3, L, D)
x0 = [320, 360, 390, 25, 60];

% Set lower and upper bounds ((P1, P2, P3, L, D)
lb = [310, 300, 300, 10, 20]; % Lower bounds for pressures and diameter
ub = [400, 400, 400, 50, 100]; % Upper bounds for pressures and diameter
```

```
options = optimoptions('fmincon', 'Display', 'iter');

% Define equality constraints (The Weymouth Relation)
P0 = 300; % psi
Pf = 400; % psi
Q = 600; % mass flow rate, MMCFD
A = 8.71 * 10^8;
Aeq = [
    (A^2)*(x0(5)^(16/3))*((x0(1)^2)-(P0^2)), -x0(4)*Q^2, 0, 0, 0;
    0, (A^2)*(x0(5)^(16/3))*((x0(2)^2)-(x0(1)^2)), -x0(4)*Q^2, 0, 0;
    0, 0, (A^2)*(x0(5)^(16/3))*((x0(3)^2)-(x0(2)^2)), -x0(4)*Q^2, 0;
    0, 0, 0, (A^2)*(x0(5)^(16/3))*((Pf^2)-(x0(3)^2)), -x0(4)*Q^2
];

beq = [0; 0; 0; 0];

% Define inequality constraints
% Maximum compression ratio K= 1.5
Aineq = [
    1.5 * P0, -x0(1), 0, 0, 0;
    0, 1.5 * x0(1), -x0(2), 0, 0;
    0, 0, 1.5 * x0(2), -x0(3), 0;
    0, 0, 0, 1.5 * x0(3), -Pf
];
bineq = zeros(4, 1);

% Perform optimization
[optimal_x, fval, exitflag] = fmincon(@Multi_Variables, x0, Aineq, bineq, Aeq,
beq, lb, ub, [], options);

disp(['P1 (psi) = ' num2str(optimal_x(1))]);
disp(['P2 (psi) = ' num2str(optimal_x(2))]);
disp(['P3 (psi) = ' num2str(optimal_x(3))]);
disp(['Length (miles) = ' num2str(optimal_x(4))]);
disp(['Diameter (inch) = ' num2str(optimal_x(5))]);
disp(['Minimum Cost function ($/yr): ' num2str(fval)]);

function f = Multi_Variables(x)
    n = 4; % number of compressors
    m = n + 1; % number of pipeline segments
    C0 = 14; % yearly operating cost $/(hp)(year)
    Cc = 70; % compressor capital cost $/(hp)(year)
    Cs = 870; % pipe capital cost $/(in)(mile)(year)
    Q = 600; % mass flow rate, MMCFD
    k = 1.26; % Cp/Cv for gas at suction conditions
    z = 0.9; % compressibility factor of gas at suction conditions
    T1 = 520; % suction temperature,°R (assumed 520°R)
    P0 = 300; % psi
    Pf = 400; % psi
    a = (z*(k-1)/k); % new constant just to simplify the objective function

    f = (C0 + Cc) * Q * 0.08531 * T1 * (k/(k-1)) * ((P0/x(1))^a +
(x(1)/x(2))^a + (x(2)/x(3))^a + (x(3)/Pf)^a - 4) + m*(Cs * x(4) * x(5));
end
```

# References


1. Armin Cosic, Michael Stadler, Muhammad Mansoor, Michael Zellinger. Mixed-integer linear programming-based optimization strategies for renewable energy communities. Journal of Renewable and Sustainable Energy, 2021, Volume 237, 1-12. DOI: 121559, https://doi.org/10.1016/j.energy.2021.121559.

2. Seyedeh Asra Ahmadi, Seyed Mojtaba Mirlohi, Mohammad Hossein Ahmadi, Majid Ameri. Portfolio optimization of power plants by using renewable energy in Iran. International Journal of Low-Carbon Technologies, May 2021, Volume 16, Issue 2, 463–475, https://doi.org/10.1093/ijlct/ctaa079.

3. Optimization of Chemical Processes, 2nd Edition; Published by McGraw-Hill Higher Education, a business unit of The McGraw-Hill Companies, Inc.; New York, NY, 2001; ISBN 0-07-039359-1.

4. Kookos, I. K. Practical Chemical Process Optimization with MATLAB and GAMS; Springer Optimization and Its Applications (SOIA), Vol. 197, 2022; pp 1-90; ISBN 978-3-031-11298-0; https://doi.org/10.1007/978-3-031-11298-0.

5. Edgar, T. F.; Himmelblau, D. M.; Bickel, T. C. Optimal Design of Gas Transmission Networks; SPE 6034; University of Texas Austin, TEX.