Dealing with Sizing operations problems for academic Education
YOUR WAY TO CHEMICAL ENGINEERING
2021 Edition

SIZING OF UNIT OPERATIONS IN PROCESS ENGINEERING

USING ASPEN HYSYS PLUS

Process Simulation Software | AspenTech

AYMEN LABIDI

Industrial Chemistry Engineering Student
National Institute of Applied Sciences and Technology

Ministry of Higher Education
and Scientific Research

Carthage University

National Institute
of
Applied Sciences and Technology

Personal Professional Project

Engineering studies

Field : **Industrial Chemistry**

Sizing of unit operations in process engineering using Aspen Hysys Plus

Presented by

Aymen Labidi

University Supervisor : **Dr Sami Abid**

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Chemical Engineering

Chemical engineering is the development of processes and the design and operation of plants in which materials undergo changes in their physical or chemical state. Applied throughout the process industries, it is founded on the principles of chemistry, physics, and mathematics.

It is the field of science that combines chemistry with technology and is able to provide solutions to most environmental problems.

Chemical Engineering covers an extremely wide range—unit operations that have played an important role in the early stages of chemical engineering, all systems and equipment in a chemical process (from raw material feed to product supply), and biotechnology and new material engineering, which are recent subjects of interest. It is said that the warp of chemical engineering comprises the means—mass transfer, energy balance, thermodynamics, transport phenomena, reaction engineering, system engineering, and so on—and its woof comprises the aims—petrochemistry, material, energy, environment, biology, and so on. However, it is not sufficient to consider chemical engineering from the viewpoint of the warp and woof, and it is expected that hybrid structures or another viewpoint will be used in the future. The probability terms and sensitiveness of human experience for quantity are missing in the definitions of the warp and woof. Nevertheless, it is no exaggeration to say that chemical engineering deals with almost all phenomena that are concerned with materials and that the domain of chemical engineering will encompass an increasingly wider range in future.

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Abstract

This project deals with the sizing of unit operations in process engineering.
Process engineering is the understanding and application of the fundamental principles and laws of nature that allow us to transform raw material and energy into products that are useful to society, at an industrial level.
By taking advantage of the driving forces of nature such as pressure, temperature and concentration gradients, as well as the law of conservation of mass, process engineers can develop methods to synthesize and purify large quantities of desired chemical products.
In this project we will focus in the design, operation, control, optimization and intensification of chemical processes by designing pipelines in each case study.
For Numerical Resolution, will use the chemical process simulator **Aspen HYSYS**, used to mathematically model chemical processes.
We have a multitude of problems to deal with during this project.

1. **Study of an incompressible fluid flow in a pipeline**

2. **Technology of Heat Exchangers**

3. **Refrigeration cycle**

Glossary

- **Q:** Volume flow.
- **HDPE:** High Density Ploy Ethylene
- **f:** friction factor
- **Re:** Reynolds Number.
- ΔH**:** Pressure Drop
- Nu **:** Nusselt Number
- **Pr:** Prandlt Number
- $\dot{Q}$**:** Heat Transfer Flow
- **U:** Overall Heat Transfer Coefficient
- $\dot{m}$**:** Mass Flow
- ΔT_{LM}**:** The logarithmic mean temperature difference
- **A:** Surface Area

About the Author

Aymen is a chemist and a simulator pilot. Born in Tunisia, he was educated at Hay El Ryadh School, El Rachidia College and Mourouj IV Hight School. Since 2018, he has studied at the **National Intsitute of Applied Science and Technology INSAT, as an Industrial Chemistry Engineering Student.**

Glider Manager for Aerobotix-INSAT and an aeronautical consultant for the FTAA, he gives onlines course session about the principle of flight and it's aerodynamic aspects.

LABIDI is the author of the Book "Quick Reference Handbook of Chemistry" for the beginner chemistry student as a 2019 edition, in 2021 he published the book in English "Sizing of Unit Operations in Process Engineering Using Aspen Hysys Plus" as a guide for process engineering operations using simulation software "Aspen Hysys Plus".

He frequently gives scientific information about chemistry and it's beauty. Since August 2019 he has published 50 research items: Papers, Research proposals, Presentations, Preprints, Articles and Technical Reports on his Research Gate profile: https://www.researchgate.net/profile/Aymen-Labidi

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I would like to express my deep gratitude and respect to M. Sami ABID, my University Supervisor, who provides me help and guidance throughout this project. Thank's for him for building the enthusiasm, critical thinking and resilience.
Also I express my thanks to my sisters for their support and valuable prayers.
Finally, my thanks go to all the people who have supported me to complete the research work directly or indirectly.

-LABIDI Aymen-

Fundamental Concepts in Chemical Engineering and Fluid Mechanics

Chemical engineers have made so many important contributions to society, in such a short span of history, that it is hard to visualize modern life without the large-scale production of antibiotics and other drugs, fertilizers, agricultural chemicals, physiological-compatible polymers for biomedical devices, high-strength polymer composites, synthetic fibers and fabrics, protective coatings, and microelectronic devices.

How would our industries function without environmental control technologies; without processes to design and make semiconductors, magnetic and optical storage media; and without modern petroleum processing?

All these technologies require the ability to produce specially-designed chemicals—and the materials based on them—economically and with minimal adverse impact on the environment. Developing this ability and implementing it on a practical scale is what chemical engineering is all about and this is what we intend to do and establish throw this project paper.

Density

The density (more precisely, the volumetric mass density; also known as specific mass), of a substance is its mass per unit volume. The symbol most often used for density is (the lower case Greek letter rho), although the Latin letter D can also be used. [2]

$$\rho = \frac{m}{v} \tag{1}$$

Viscosity

The viscosity of a fluid is a measure of its resistance to deformation at a given rate. For liquids, it corresponds to the informal concept of "thickness", it can be conceptualized as quantifying the internal frictional force that arises between adjacent layers of fluid that are in relative motion. We can define the **Dynamic viscosity** and **Kinematic Viscosity**[3]

Reynolds Number

The Reynolds number (Re) helps predict flow patterns in different fluid flow situations. At low Reynolds numbers, flows tend to be dominated by **laminar** flow (Re<2000), while at high Reynolds numbers flows tend to be **turbulent** (Re>3000).

$$Re = \frac{D\ v\ \rho}{\mu} \tag{2}$$

Where:

- ρ- Fluid Density
- μ- Dynamic Viscosity
- v-Velocity
- D-Diameter

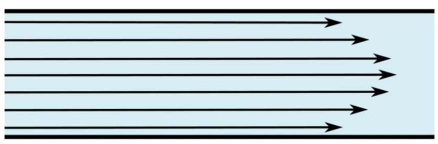


Figure 1 – Laminar Flow

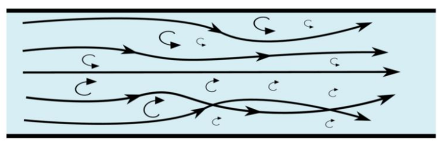


Figure 2 – Turbulent Flow

Pressure Drop

Pressure drop is defined as the difference in total pressure between two points of a fluid carrying network. A pressure drop occurs when frictional forces, caused by the resistance to flow, act on a fluid as it flows through the tube.

Bernoulli's Principle

In fluid dynamics, Bernoulli's principle states that an increase in the speed of a fluid occurs simultaneously with a decrease in static pressure or a decrease in the fluid's potential energy [4] The principle is named after Daniel Bernoulli who published it in his book Hydrodynamica in 1738.The principle is only applicable for isentropic flows: when the effects of irreversible processes (like turbulence) and non-adiabatic processes.

$$\frac{1}{2}\ \rho v^2 + \rho g z + p = constant \tag{3}$$

Chapter I

Study of an incompressible fluid flow in a pipeline

Introduction

We desire to deliver water at a rate of 150 m^3/h from point (A) to point (B) through a **HDPE (High Density Polyethylene) PN10 pipe**.
The distance between points (A) and (B), assumed to be horizontal, is **L=500 m**.

Our task consists of **proposing a suitable diameter** for pipeline and determine the **output pressure** P_B**.**

- Water Temperature is 30 °C
- Pressure at point A is 2.5 bar
- Two 45 °elbows
- Gate Valve (Direct-pass valve - Full open)

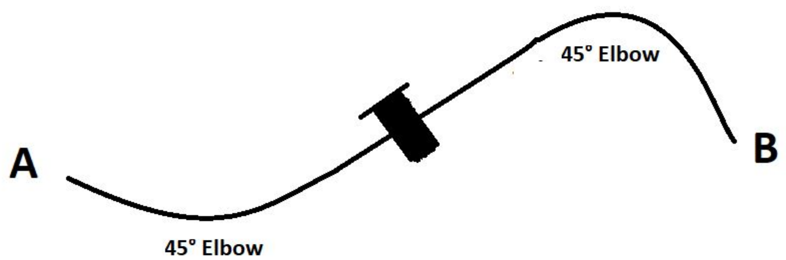


Figure I.1 – Problem Presentation Design

1 Problem Resolution using Excel

1.1 Fluid Characteristics

The physical properties of water were selected from the *CRC Handbook of Chemistry and Physics*

Table I.1 – Characteristics of the Fluid at 30 °C

Fluid	Water
Volume Flow (m^3/s)	0,041666666
Gravity Field (m/s^2)	9,81
Density (kg/m^3)	998
Dynamic Viscosity (Pa.s)	$7{,}977.10^{-4}$
Kinematic Viscosity (m^2/s)	$8{,}01185.10^{-7}$

1.2 Pipe Characteristics

High-density polyethylene (HDPE) or polyethylene high-density (PEHD) is a thermoplastic polymer produced from the monomer ethylene. It is sometimes called "alkathene" or "polythene" when used for HDPE pipes [5] With a high strength-to-density ratio, HDPE is used in the production of plastic bottles, corrosion-resistant piping, geomembranes and plastic lumber. HDPE is commonly recycled, and has the number "2" as its resin identification code.

Figure I.2 – HDPE has SPI resin ID code

1.3 Theoretical Pressure Drops using Coleboork White Method

1.3.1 Singular Pressure Drops

We used Excel (Check File with this project) to estimate the value of elbow's and valve's coefficients (K_i) and to calculate the total **Singular pressure drop**.
NOTE: We have chosen to use a gate valve with a nominal Diameter of 4"

Table I.2 – Singular Pressure Drop

Quantity	2	1
Type	elbow	Gate Valve
Angle (°)	45	180
K_i	1,086	10
K	6,486	

In order to calculate the Pressure drop coefficient K_i of the elbows, we used the expression below: (Check Excel paper)

$$K_i = \sin^2 \alpha + 2 \sin^4 \frac{\alpha}{2} \tag{I.1}$$

Where α is the elbow's angle ($\alpha = 45°$ in our case)
So, we can now estimate the **singular pressure drop** ΔH_s using this expression:

$$\Delta H_s = \frac{Kv^2}{2g} \tag{I.2}$$

Where

- v: The Flow Velocity (m/s)
- g: The Gravity Field

But how could we estimate the velocity ?
To calculate the velocity, we should use the expression below

$$v = \frac{4\ Q_v}{\pi\ D^2} \tag{I.3}$$

Where

- Q_v is the volume flow
- D: The pipe Diameter (that we should estimate)

NOTE:
The Fluid velocity into the pipe should be lower than 1.5 $m/\ s$ **to avoid the temperature rise and noisy flow and greater than 0.65** $m/\ s$ **to avoid the sedimentation**
Check the Excel file to see that we find an **adequate velocity of 1.044 m/s** using a **Diameter of 0.22540086601865 m**
So, Estimated **Singular Pressure** Drop will be:

$$\Delta H_s = 59.290\ m \tag{I.4}$$

1.3.2 Regular Pressure Drops

To start with, we should provide a value of the Diameter (hypothetical value), this is not arbitrary !
We have already provided an **Internal Diameter estimation of 0.22540086601865 m**
Now, we are going to search the friction factor "f", the value we should assume must verify the **Colebrook equation**, it means that the with the chosen value of the friction factor, the Colebrook equation **should be equal to zero or almost (because it could not be exactly equal to zero as we are modifying a lot of parameters at one time)**
The Colebrook White equation is:

$$\frac{1}{\sqrt{f}} = -2\log[(\frac{e}{3.7D}) + \frac{2.51}{Re\ \sqrt{f}}] \tag{I.5}$$

Where

- f- friction factor
- D- Pipe inside Diameter
- e- absolute pipe roughness
- Re- Reynolds number of flow

Reynolds number could be calculated using this Formula:

$$Re = \frac{D\ v\ \rho}{\mu} \tag{I.6}$$

Where:

- ρ- Fluid Density
- μ- Dynamic Viscosity

As for our **High Density Polyethylene Pipe**, the Absolute roughness is: $e = \ 1.52\ 10^{-6}\ m$ (Please Check Excel File to understand the calculation approach.)

Steps to follow using Excel Solver Feature

- Go under DATA
- Select What-if Analysis
- Proceed to Goal Seek
- Under "Set Cell", select the Colebrook Equation cell
- Set the value "0" in "To Value" option
- Finally, select the Friction factor cell under "By changing cell"

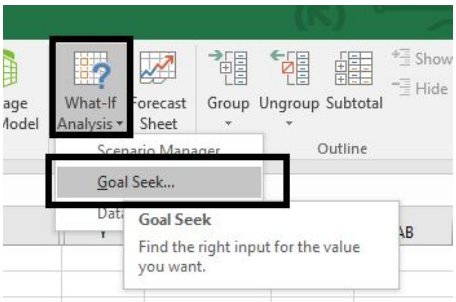


Figure I.3 – Solver steps

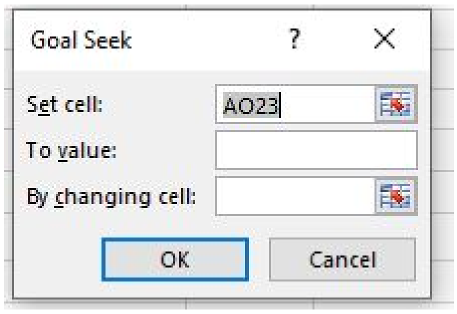


Figure I.4 – Goal Seek Cells settings

Resolving the Colebrook Equation, we find a **friction factor of 0.0145903975287305**
At this stage, we can calculate the regular pressure drops using the expression below:

$$\Delta H_r = \frac{fv^2L}{2gD} \tag{I.7}$$

So, after calculation, we had:

$$\Delta H_r = 1.799\ m \tag{I.8}$$

1.3.3 Theoretical Values

Below, we provide a summary table:

Table I.3 – Summary Table -1-

Parameter	Value
Diameter(m)	**0.225400866**
velocity(m/s)	1.044
Reynolds	2.93 10^5
Friction Factor	0.0145903975287305
ΔH_s (m)	59.290
ΔH_r (m)	1.799
ΔH_t (m)	61.089

As We can see, we have estimated the theoretical value for the internal pipe Diameter, but we should check the commercial catalog provided for internal diameters.
From all given values, we choose Closest three values to our calculated internal diameter.
But, From these three Commercial values, we should choose the one having a velocity of around the 1 m/s.
To do this, we calculated the velocity for each given diameter, results are on the table below:

Table I.4 – Internal Diameter Choice

Commercial Diameter(mm)	Thikness (mm)	Internal Diameter (mm)	Velocity (m/s)
250	14.8	220.4	1.092133401
315	18.7	277.6	0.688430252
400	23.7	352.6	0.426711408

The Only value inline with our approach is the first one (blue), so we can choose a **Commercial Diameter of 250 mm** for which corresponds an **internal Diameter of 220.4 mm**

1.4 Outlet Pipeline Pressure

The pressure calculation is based on the famous **Bernoulli's Principle**

$$\frac{v_A^2 - v_B^2}{2g} + \frac{P_A - P_B}{\rho g} + (Z_A - Z_B) = \Delta H_t \quad (m) \tag{I.9}$$

We should pay attention to the unit conversion !!
Reminds:
1 bar = 1.01325 . $10^5 Pa$

In the table below, we present our results:

Table I.5 – Pressure Result using Colebrook White Method

Size	Velocity (m/s)	Pressure (bar)	Height
Point A	1.044	2.5	Same as B
Point B	1.044	2.49	Same as A

2 Equivalent Lengths Method for Total Pressure Drop Calculation

Before switching to the simulation calculation, let's check another time our Hand calculations using this precious **Equivalent Length method**.
What's the Equivalent Length method ?
The equivalent length method (L/D ratio) allows the user to describe the pressure drop through a fitting as a length of pipe. In theory the pressure drop through the fitting is equivalent to

the pressure lost through a certain length of piping at that corresponding flow rate.

So we will need a chart in **Appendix** 1 shown in III, and we will use segments strating from our diamemter (which is 225 mm and outer of 250 mm) and toward our singulatrities, these segments are crossing the horizental axis of equivalent lengths (in meters), so here we note the our equivalent length value for each singulatrity.
As you can see the red arrow is standing fro the 45 °elbows and orange arrow for the open valve (Gate valve).

so we find:
$L_{Eq-45Elbow} = 7\ m$ **and** $L_{Eq-valve} = 1.8\ m$
as a result the Total Equivalent Length is assumed to be:
$L_{Eq-Tot} = 500 + (7 * 2) + 1.8 = 515.8\ m$

In order to calculate the total pressure drop, we don't need to calculate the singular pressure drop as in the previous method because we have substituted the singulatrities with their equivalent lengths in the linear pressure drop, which is the total pressure drop, we have to use this formula:

$$\Delta H_{Tot} = \lambda \frac{v^2}{2gD} L_{éq-Tot} \quad (m) \tag{I.10}$$

Hand calculation gives us:

$$\Delta H_{Tot} = 0.0146 * \frac{1.04^2}{2 * 0.255 * 9.81} * 515.8 = 1.628027321\ m \tag{I.11}$$

PLEASE PAY ATTENTION to the unit used here (m, we should convert it to bar
To do this, just multiply it by ρg, you will get a value with **Pascal**, then divide it by $1.01325\ .10^5$
Below a summary table using this the **Equivalent Length method**

Table I.6 – Summary Table -2-

Parameter	Value
Diameter(m)	**0.225400866**
velocity(m/s)	1.044
Reynolds	2.93 10^5
Friction Factor	0.0145903975287305
$L_{éq-coude45}$ (m)	7
$L_{éq-vanne}$ (m)	1.8
$L_{éq-Tot}$ (m)	515.8
ΔH_{Tot} (bar)	0.179

Now, using the **Bernoulli's Principle** as mentioned in (I.9) we calculate the Outlet Pressure P_B.

Table I.7 – Pressure Result using Equivalent Lengths Method

Size	Velocity (m/s)	Pressure (bar)	Height
Point A	1.044	2.5	Same as B
Point B	1.044	2.321*	Same as A

* How calculation was proceeded ?
Points A and B have the same velocity and the same Height, so in **Bernouilli's Principle Equation**, we will have only the pressure to consider.

$$P_A - P_B = \Delta H_{Tot} \tag{I.12}$$

$$P_B = \frac{((2.5 * 1.01325 * 10^5) - (0.179 * 1.01325 * 10^5))}{1.01325 * 10^5} = 2.321\ bar \tag{I.13}$$

2.1 Synthesis

Based on Excel calculation using the two methods, we can conclude that:

- Internal Diameter = 220.4 mm but we will consider it as 225 mm
- Outlet Pressure = 2.49 bar using Colebrook Method
- Outlet Pressure = 2.321 bar using Equivalent Lengths Method

As we can see, the values of the Outlet Pressure are almost the same, this little difference is due to the precision of the second method.

3 Colebrook resolution using MATLAB

3.1 What is MATLAB ?

MATLAB (" matrix laboratory ") is a scripting language [6] emulated by a development environment of the same name; it is used for numerical calculation purposes . Developed by The MathWorks company , MATLAB allows you to manipulate matrices, display curves and data, implement algorithms, create user interfaces, and can interface with other languages such as C , C ++ , Java , and Fortran . MATLAB users (around 4 million in 2019 [7]) are from very different backgrounds such as engineering, science and economics in an industrial context as well as for research. Matlab can be used alone or with toolboxes .

The main goal of SRE is to create, maintain and evolve a scalable and highly reliable infras-

Figure I.5 – MATLAB Logo

tructure to support the ever-growing demands of modern software applications.

3.2 Friction Factor Determination

In order to calculate the friction factor, we should first define the Reynolds Number function. Under ***"ReynoldsNumber.m"*** we developed this script:

```
function [Re] = ReynoldsNumber(density,velocity,diameter,viscosity)
Re= density*velocity*diameter/viscosity;
end
```

```
>> ReynoldsNumber(rho, V, D, mu)

ans =

   2.9371e+05
```

Figure I.6 – Reynolds Number result

We can now, calculate the friction factor using this developed script under ***"colebrook.m"***

```
function F = colebrook(R,K)
if any(R(:)<2300) == 1,
warning('The Colebrook equation is valid for Reynolds" numbers >= 2300.');
end,
if nargin == 1 || isempty(K) == 1,
K = 0;
end,
if any(K(:)<0) == 1,
warning('The relative sand roughness must be non-negative.');
end,
X1 = K .* R * 0.123968186335417556;
X2 = log(R) - 0.779397488455682028;
F = X2 - 0.2;
E = ( log(X1+F) - 0.2 ) ./ ( 1 + X1 + F );
F = F - (1+X1+F+0.5*E) .* E .*(X1+F) ./ (1+X1+F+E.*(1+E/3));
E = ( log(X1+F) + F - X2 ) ./ ( 1 + X1 + F );
F = F - (1+X1+F+0.5*E) .* E .*(X1+F) ./ (1+X1+F+E.*(1+E/3));
F = 1.151292546497022842 ./ F;
F = F .* F;
```

The friction factor is shown below, almost equal to the one found by Excel

```
>> colebrook(2.93*10^(5),1.52*10^(-6))

ans =

    0.0145
```

Figure I.7 – Friction factor estimation using matlab

3.3 Synthesis

As you can see, the friction factor we had using matlab is exactly the same we had using the Excel Approach, but we should say that Matlab is so far simplifying the calculation task throw functions used in the script above, the precision, speed and effectiveness of calculation process is what we are chasing.

4 Aspen Hysys Simulation

4.1 Simulation Process

We Will proceed to simulation using the latest version of Aspen Hysys (Aspen Hysys V.11) Below; we are developing the detailed steps to follow in order to succeed your simulation process.

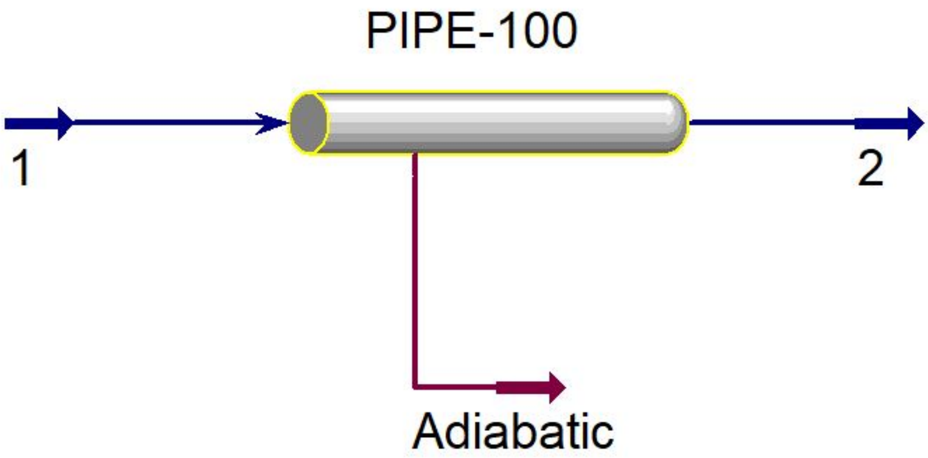


Figure I.8 – Pipe Precess Design

- After Opening ASPEN HYSYS 11, under **Properties - Component lists** define your fluid which is the **Water** in our case.

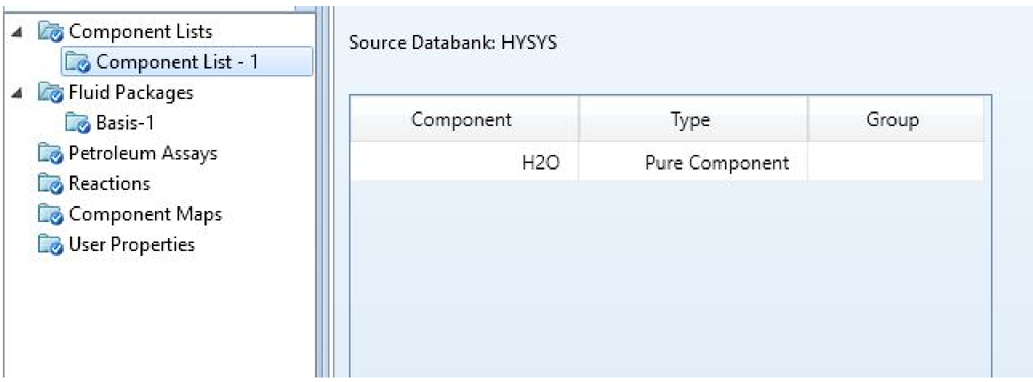


Figure I.9 – Fluid selection

- Go to **Fluid Packages**, then choose the **Peng-Robinson** package which is usually used for hydrocarbons.

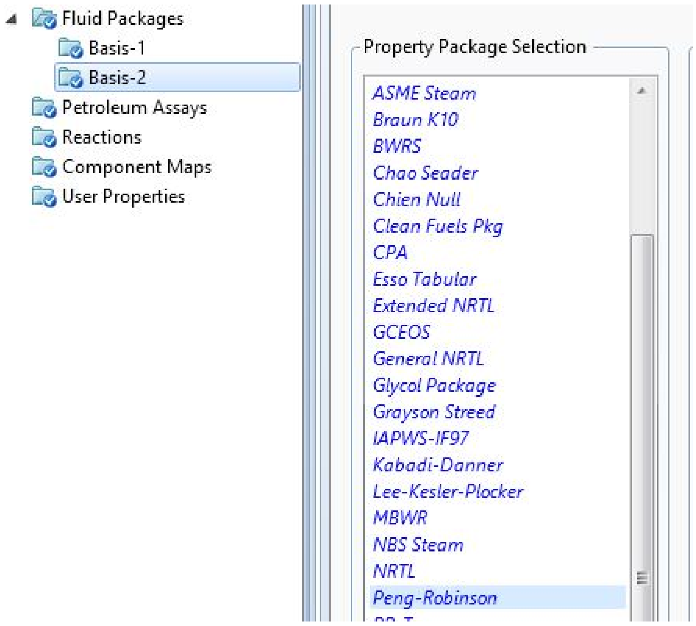
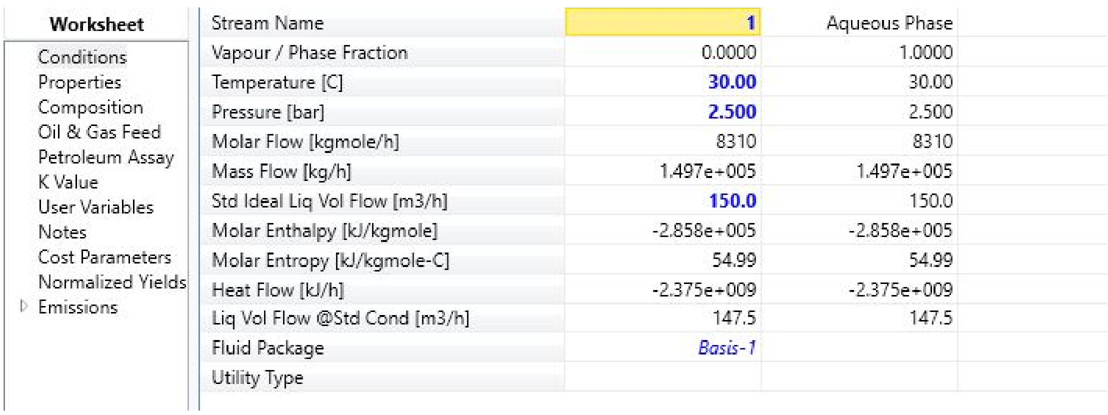


Figure I.10 – Fluid package selection

- Now, you can proceed to **Simulation** which is the option after **properties**: As a first step, we should define our **Inlet Material Stream** entering the problem **Temperature** which is 30 ℃, the **Inlet Pressure** of 2.5 bar and the **Liquid Volume Flow of 150** m^3/h



Stream Name	1	Aqueous Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	30.00	30.00
Pressure [bar]	2.500	2.500
Molar Flow [kgmole/h]	8310	8310
Mass Flow [kg/h]	1.497e+005	1.497e+005
Std Ideal Liq Vol Flow [m3/h]	150.0	150.0
Molar Enthalpy [kJ/kgmole]	-2.858e+005	-2.858e+005
Molar Entropy [kJ/kgmole-C]	54.99	54.99
Heat Flow [kJ/h]	-2.375e+009	-2.375e+009
Liq Vol Flow @Std Cond [m3/h]	147.5	147.5
Fluid Package	Basis-1	
Utility Type		

Figure I.11 – Defining Inlet Worksheet

- You should go to **Composition** menue and fill the **LiqVol Flows** and **Mass Fractions** with respectively 150 and 1.

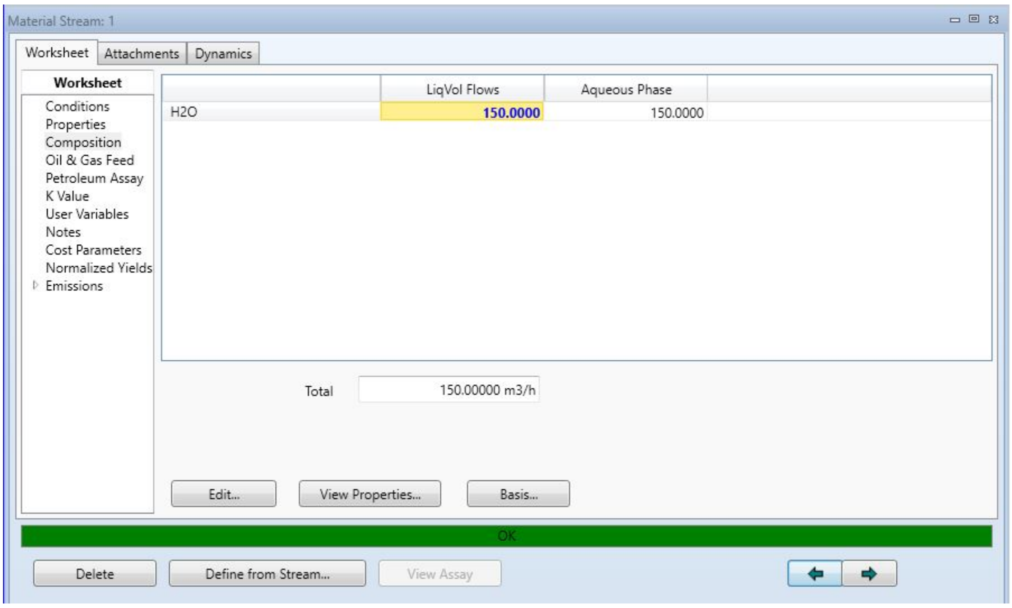


Figure I.12 – Defining The Fluid Composition in the Inlet Stream

- in the **Model Palette** choose the **Pipe Segment** to define our pipeline, then we should define the Inlet of the pipe, the Outlet is called "2" and we should give an **Energy Stream** called "Adiabatic"

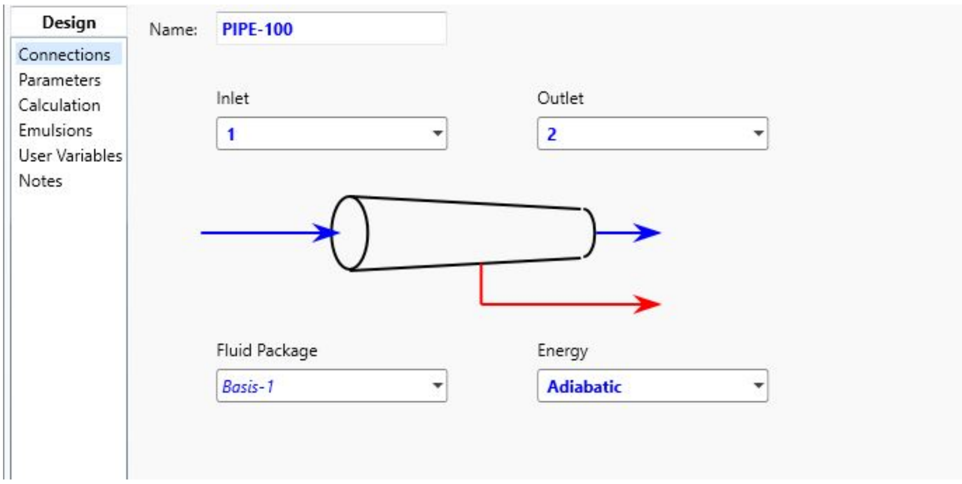


Figure I.13 – Defining the Pipe segment

- Now, we should go to the **Rating** option, click on **Append Segment** then then fill it with the required information, we will use **Equivalent Length** to enter our equivalent Length of 515.8 m and don't forget to define pipe roughness.
- As for Heat Transfer, we will consider it as zero, which means an **Adiabatic Transfer**,

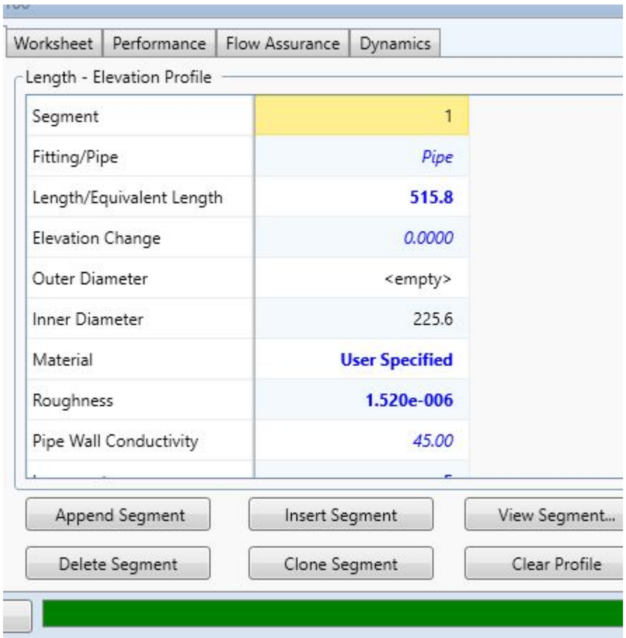


Figure I.14 – Sizing the Pipe segment

to do that, select Heat Transfer under the Sizing Option and put it as Zero.

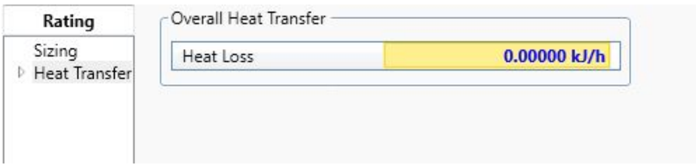


Figure I.15 – Rating Heat Transfer into the the Pipe segment

- Now, go and select **Outlet Flow** then **Attachments** and select **Analysis** to introduce **Line-Sizing Manager** and then select the Velocity Criteria, we will admet it bteween 1-2 m/s. (1.1 m/s)

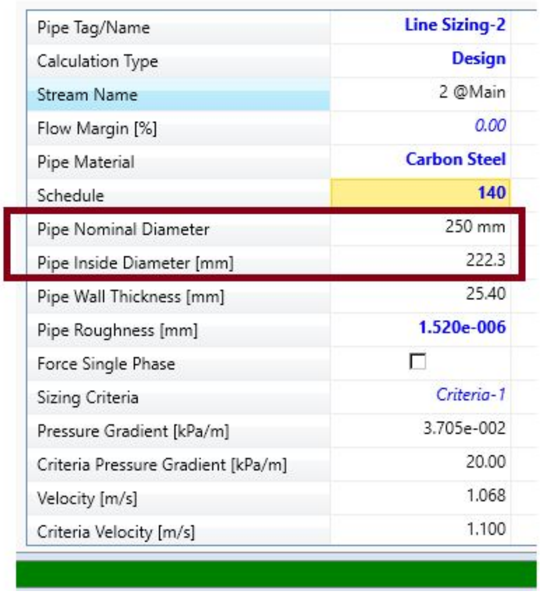


Figure I.16 – Line Sizing Manager

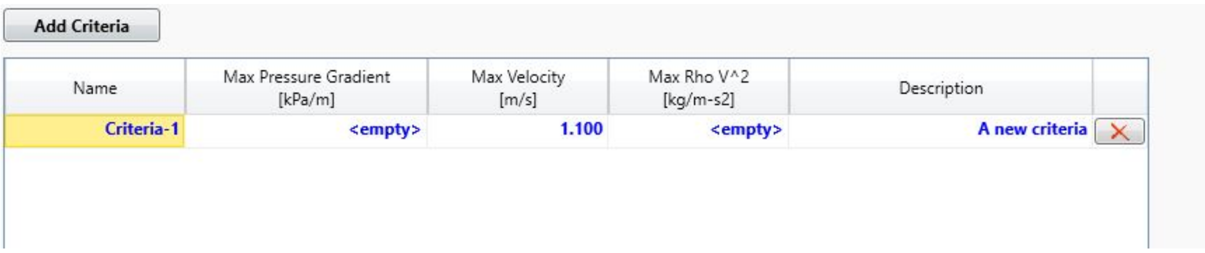


Figure I.17 – Entering the Velocity Criteria

In this step, Aspen will use it's solver algorithm to calculate a suitable diameter for our pipe as well as the pressure at Point B, o as you can see we have an **Inner Pipe Diameter of 222.3 mm** which is pretty close to the one calculated manually.**(Note that this is the most near diameter allowed by Aspen in this category to the one hand calculated)** Also, the Calculated **pressure in the Outlet Stream Material is exactly 2.3 bar** and we should say that's very close to the value we have calculated which is **2.321**(Please see the Video Included in this Project)

Segment	1
Fitting/Pipe	*Pipe*
Length/Equivalent Length	**515.8**
Elevation Change	*0.0000*
Outer Diameter	273.1
Inner Diameter	222.3
Material	**PlasticTubing**
Roughness	**1.400e-005**
Pipe Wall Conductivity	**0.1700**
Increments	**5**
FittingNo	<empty>

Figure I.18 – Calculating the Suitable Diameter

Stream Name	2	Aqueous Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	30.00	30.00
Pressure [bar]	2.300	2.300
Molar Flow [kgmole/h]	8310	8310
Mass Flow [kg/h]	1.497e+005	1.497e+005
Std Ideal Liq Vol Flow [m3/h]	150.0	150.0
Molar Enthalpy [kJ/kgmole]	-2.858e+005	-2.858e+005
Molar Entropy [kJ/kgmole-C]	55.00	55.00
Heat Flow [kJ/h]	-2.375e+009	-2.375e+009
Liq Vol Flow @Std Cond [m3/h]	147.5	147.5
Fluid Package	*Basis-1*	
Utility Type		

OK

Figure I.19 – Calculating the Outlet Pressure in the Pipe

Now, in order to better visualize the pressure drop with pipe length, we proceed to the data Performance and we can consult the pressure table as seen below and the Plot we get shows exactly how the pressure is dropping and decreasing along the pipe Length. In this figure you can **Clearly** see that the pressure in the last point of the pipe is **2.3 bar** which is so close to **2.321 bar** (the one calculated manually)

In Table I.8 we compare our simulation results with the analytical ones.

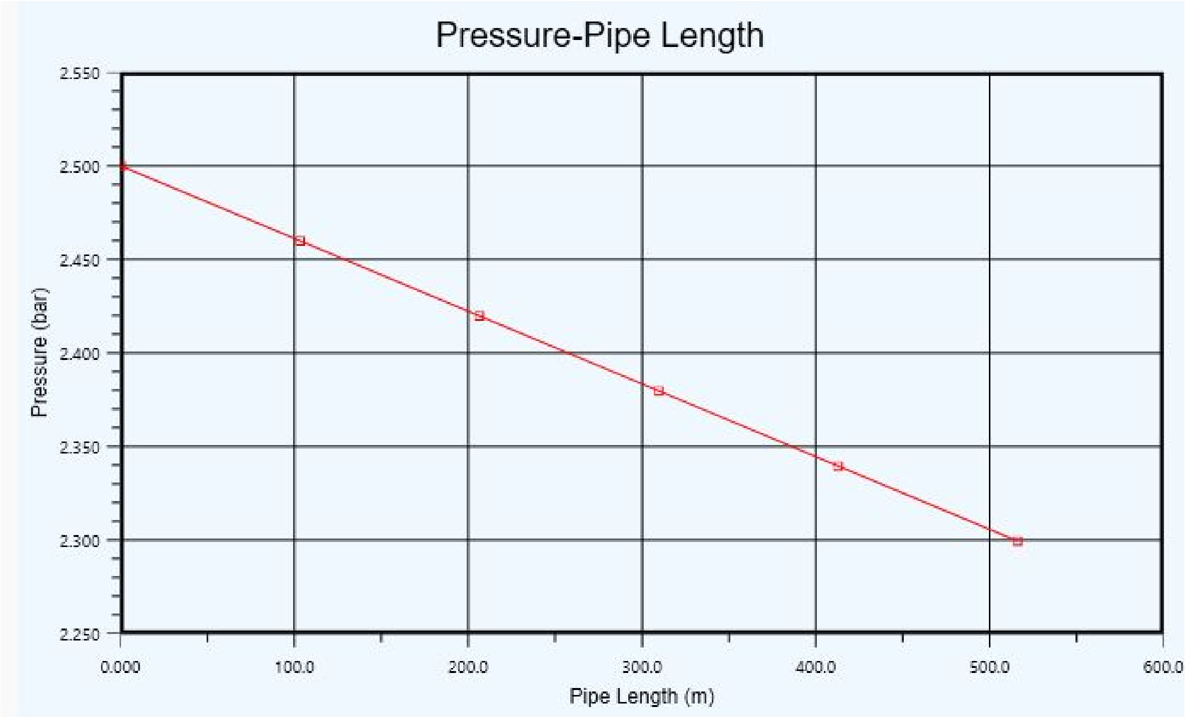


Figure I.20 – Plot of the pressure drop along the pipe length

Length [m]	Elevation [m]	Pressure [bar]
0.000	0.000000	2.50000
103.160	0.000000	2.45992
206.320	0.000000	2.41984
309.480	0.000000	2.37976
412.640	0.000000	2.33968
515.800	0.000000	2.29960

Figure I.21 – Table showing the variation of pressure with pipe Length

Table I.8 – Summary Table -3-

Parameter	Hand Calculation	Simulation Calculation
Diameter(mm)	**225,400866**	**222.3**
velocity(m/s)	1.044	1.068
ΔH_{Tot} (bar)	0.179	0.1911
Outlet Pressure (bar)	**2.321**	**2.300**

But Now, What about using the Singularities Option in the Simulator Aspen ?

After Loading your **Component List** and **Fluid Package**, you define your **Inlet Stream** as in I.11 figure.
Below the Steps to follow:

1. Add your Pipe Segment from the Model Palette

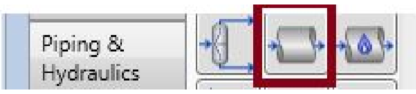


Figure I.22 – Pipe segment - Model Palette

2. Define your Inlet, Outlet and Energy Stream, for sure it's and **Adiabatic** transformation, so you define your Energy stream as 0 the same as mentioned in Figure I.13 and I.15

3. Now, proceed to **Rating** Option, then select **Sizing** and here we should introduce all Pipe Data: (**Without Forgetting your Inner Diameter of 225 mm)**

   - Pipe Segment
   - 2 x Elbow of 45 °std
   - Gate Valve: Fully open

   See Figure I.23

Length - Elevation Profile

Segment	1	2	3	4
Fitting/Pipe	Pipe	Elbow: 45 Std	Elbow: 45 Std	Gate Valve: Open
Length/Equivalent Length	500.0	2.613	2.613	2.337
Elevation Change	0.0000	0.0000	0.0000	0.0000
Outer Diameter	250.0	<empty>	<empty>	<empty>
Inner Diameter	225.0	225.0	225.0	225.0
Material	PlasticTubing	PlasticTubing	PlasticTubing	Mild Steel
Roughness	1.400e-005	1.400e-005	1.400e-005	4.572e-005
Pipe Wall Conductivity	0.1700	0.1700	0.1700	45.00
Increments	5	1	1	1
FittingNo	<empty>	1	1	1

Figure I.23 – Pipe Segment - Rating and Sizing

4. Define your Heat Transfer as **0 Kj/h** in the **Heat Transfer Section**

5. As We have already mentioned that our process will be **adiabatic** and that the temperature in the Inlet Stream is 30 °C so Aspen will calculate automatically your **Pressure Drop**. To get your calculated value, under **Pipe Segment PIPE-100 - Design - Parameters**, you will find $\Delta P = 18.58\ kPa = 0.1858\ bar$

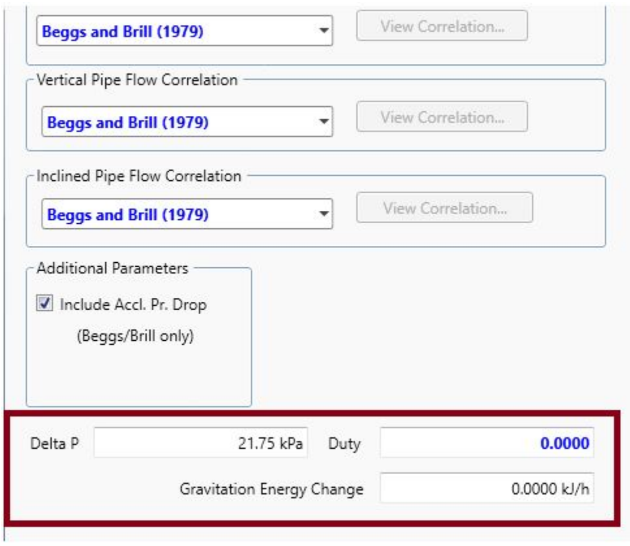


Figure I.24 – Pressure Drop Estimation by Aspen

6. Now, let's check the **Outlet Pressure** (pressure at point B).
   To do this, just click on the Outlet Stream **"2"** (Which should be in **Dark Blue** **(Full Given Data for pressure calculation)**). So as you can see in Figure I.26 the **Outlet pressure is 2.314 bar** (The one Hand Calculated was **2.321 bar**)

Stream Name	2	Aqueous Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	30.00	30.00
Pressure [bar]	2.314	2.314
Molar Flow [kgmole/h]	8310	8310
Mass Flow [kg/h]	1.497e+005	1.497e+005
Std Ideal Liq Vol Flow [m3/h]	150.0	150.0
Molar Enthalpy [kJ/kgmole]	-2.858e+005	-2.858e+005
Molar Entropy [kJ/kgmole-C]	55.00	55.00
Heat Flow [kJ/h]	-2.375e+009	-2.375e+009
Liq Vol Flow @Std Cond [m3/h]	147.5	147.5
Fluid Package	Basis-1	
Utility Type		

OK

Figure I.25 – Outlet Pressure Estimation by Aspen

7. We have plotted the **pressure-Pipe Length curve**, you can clearly see an outlet pressure of 2.314 bar approximately

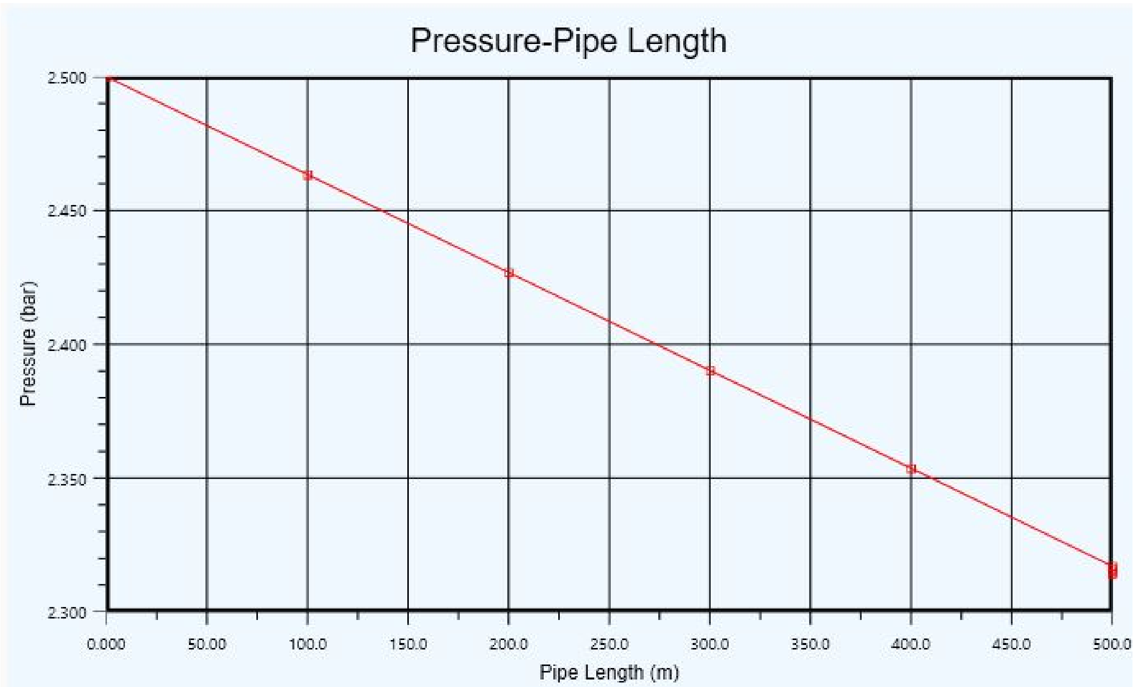


Figure I.26 – Pressure-Pipe Length Plot

4.2 Synthesis

Table I.9 – Summary Table -4-

Parameter	Hand Calculation	Simulation Calculation
Diameter(mm)	**225,400866**	**222.3**
velocity(m/s)	1.044	1.068
ΔH_{Tot} (bar)	0.179	0.1858
Outlet Pressure (bar)	**2.321**	**2.314**

In the table I.9 we summarize the simulation results with those hand calculated.
We find that the results are approximately the same (close results) The results are so close, so we can adopt this approach in the simulation process.
As a result, we can say that the two approaches: Singularities Option and Equivalent Length method are satisfying in term of results.
But, when we Introduce the real Problem Singularities, Aspen provide us with a more slightly precise value.

Chapter II

Technology of Heat Exchangers

Contents

Introduction

This chapter will go over the technology of **Heat Exchangers** and their design using chemical Engineering simulation.However, before diving deeper, it is imperative to give an overview of the theory of heat exchanger in relation to heat transfer.

1 Heat Exchanger

1.1 What's a Heat Exchanger ?

A **heat exchanger** is a device for transferring thermal energy from one fluid to another without mixing them. The heat flow passes through the exchange surface which separates the fluids [8]. The advantage of the device lies in the separation of the two circuits and in the absence of other exchanges than heat, which keeps the physicochemical characteristics (pressure, concentration of chemical elements, etc.) of each fluid unchanged except for their temperature. or their condition .

An exchanger is characterized by the fluids present, the desired goal and the power to be used; these criteria determine its optimal shape and dimensions.

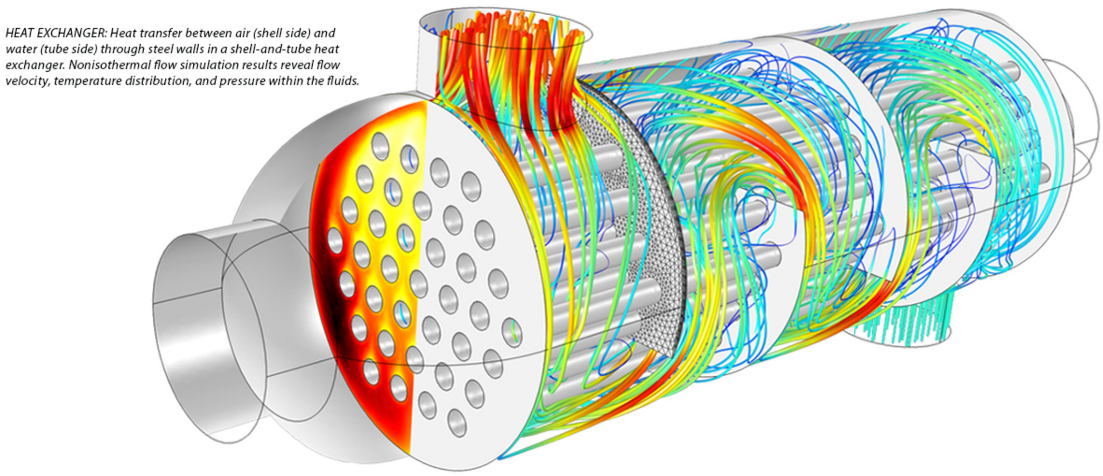


Figure II.1 – Simulation of Heat Exchangers

1.2 Use of Heat Exchangers

Heat exchangers are used in many fields and have a number of applications, such as:

- **the boiler** , the heat exchangers can be produced by water heated by recovering the energy of the combustion products;
- **the radiators** apartments allow, with water heaters, heat the air of the premises where they are installed for our comfort;
- **the refrigerating machine** , be it a refrigerator , an air conditioner or a heat pump , where they are needed;
- **the cooling of hot fluids**, to avoid damage due to a too high temperature; this is the typical case of the automobile radiator;

1.3 Types of Heat Exchangers

Different types of exchangers adapt to the desired objectives.

- **U-tube heat exchanger**
  This is the most common exchanger. In this same catergory, we can find the **Horizental**

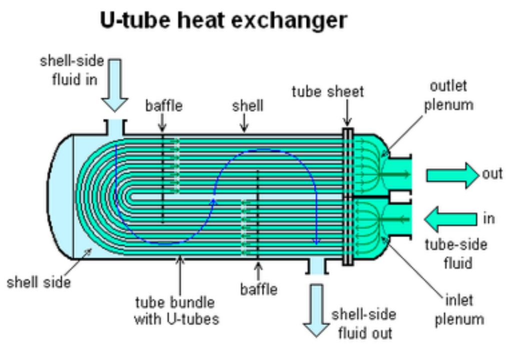


Figure II.2 – Diagram of a U-tube heat exchanger.

tube bindle exchanger and the **Vertical tube bundle heat exchanger**

- **Spiral Exchanger**
  A spiral heat exchanger consists of 2 metal plates helically wound to form a pair of spiral channels

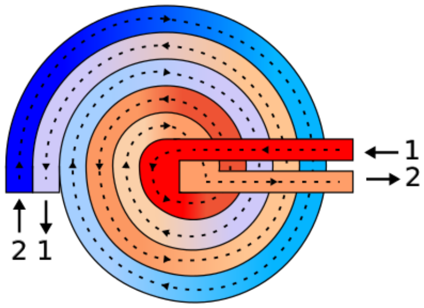


Figure II.3 – Diagram of a spiral exchanger.

- **Plate heat exchanger**
  It's a famous one.The plate exchanger is a type of heat exchanger which is experiencing increasing use in industry and in climate engineering . It is made up of a large number of plates arranged in the shape of a millefeuille and separated from each other by a space of a few millimeters where the fluids circulate.

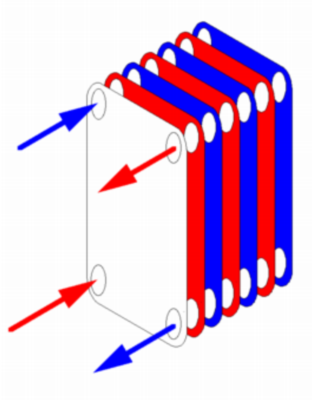


Figure II.4 – Diagram of a plate heat exchanger

- **Column of Bouhy**
  An excellent alternative to plate exchangers in compressed air dryers , the Bouhy column is in fact a pinhead exchanger to which a centrifugal air / water separator has been added in the lower part. The device has two coaxial exchangers, the first serving to bring the air below its dew point , the second serving both to bring the air to a temperature suitable for its use and above all to increase the efficiency of the cooling.

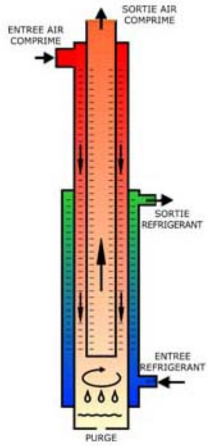


Figure II.5 – Column of Bouhy.

- **Block heat exchanger**
  The block exchanger is a type of heat exchanger reserved for particular applications. It consists of a block of a thermally conductive material pierced with multiple channels in which the 2 fluids circulate.

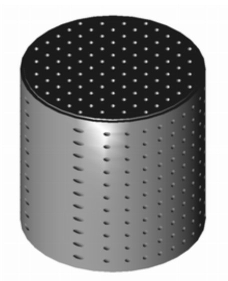


Figure II.6 – Diagram of a single block heat exchanger.

- **Finned heat exchanger**
  A finned heat exchanger is a relatively simple heat exchanger: it consists of a cylindrical or rectangular duct on which metal strips of different shapes are fixed. The coolant is generally ambient air. The heat is transferred from the hot fluid circulating in the main duct to the metal blades by thermal conduction ; these blades cool on contact with air.

Figure II.7 – Automotive water / air exchanger..

2 Fundamental Concepts of Heat Transfer

2.1 Transfer modes

Heat flows across temperature differences. There are *three modes* of heat transfer:

- **Conduction** is an exchange of energy by direct interaction between molecules of a substance containing temperature differences. It occurs in gases, liquids, or solids and has a strong basis in the molecular kinetic theory of physics.

- **Convection** may be described as conduction in a fluid as enhanced by the motion of the fluid. It may not be a truly independent mode, but convection is the most heavily studied problem in heat transfer: More than three-quarters of all published heat transfer papers deal with convection. This is because convection is a difficult subject, being strongly influenced by geometry, turbulence, and fluid properties.

- **Radiation** is a transfer of thermal energy in the form of electromagnetic waves emitted by atomic and subatomic agitation at the surface of a body.

Conduction and radiation are fundamental physical mechanisms, while convection is really conduction as affected by fluid flow.

2.2 Logarithmic Temperature Difference

The **logarithmic mean temperature difference (also known as log mean temperature difference, LMTD)** is used to determine the temperature driving force for heat transfer in flow systems, most notably in heat exchangers. The LMTD is a logarithmic average of the temperature difference between the hot and cold feeds at each end of the double pipe exchanger. For a given heat exchanger with constant area and heat transfer coefficient, the larger the LMTD, the more heat is transferred. The use of the LMTD arises straightforwardly from the analysis of a heat exchanger with constant flow rate and fluid thermal properties.

We assume that a generic heat exchanger has two ends *(which we call "A" and "B")*, please see **Figure** II.8 at which the hot and cold streams enter or exit on either side; then, the LMTD is defined by the logarithmic mean as follows:

$$LMTD = \Delta T_{LM} = \frac{\Delta T_A - \Delta T_B}{\log(\frac{\Delta T_A}{\Delta T_B})} = \frac{\Delta T_A - \Delta T_B}{\log(\Delta T_A) - \log(\Delta T_B)} \qquad \text{(II.1)}$$

where ΔT_A is the temperature difference between the two streams at end A, and ΔT_B is the temperature difference between the two streams at end B.

With this definition, the ΔT_{LM} can be used to find the exchanged heat in a heat exchanger:

$$Q = U * A * \Delta T_{LM} \quad (Watt) \qquad \text{(II.2)}$$

Where Q is the exchanged heat duty, U is the heat transfer coefficient (in watts per kelvin per square meter) and A is the exchange area. Note that estimating the heat transfer coefficient may be quite complicated.

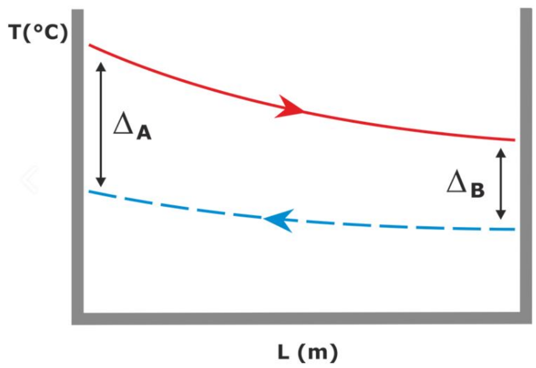


Figure II.8 – The LMTD illustrated in a countercurrent temperature profile [1]

3 The Condensation of a Steam in a Condenser

3.1 Problem Introduction

Steam in the condenser of a power plant is to be condensed at a temperature of **30 °C** with cooling water from a nearby lake, which enters the tubes of the condenser at **14 °C** and leaves at **22°C**. The surface area of the tubes is 45 m^2, and the overall heat transfer coefficient is $2100 W/m^2$°**C.**

Our Task consists on Determining the mass flow rate of the cooling water needed and the rate of condensation of the steam in the condenser

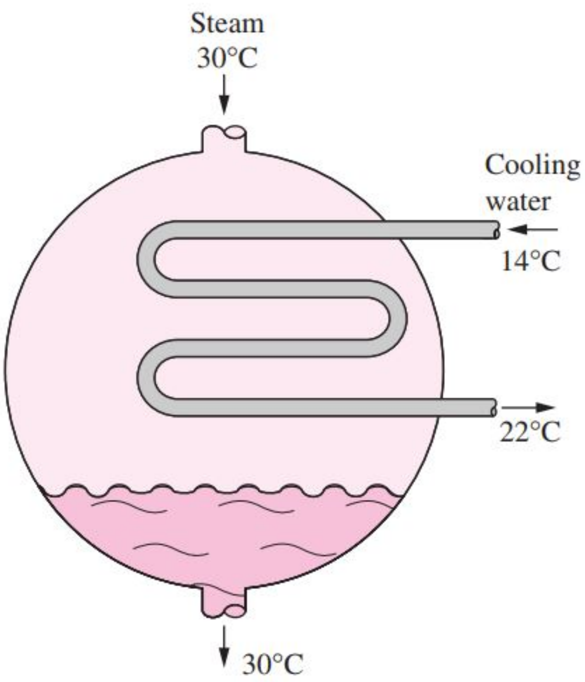


Figure II.9 – Schematic representation of a Boiler for our Problem

Fluid	Water
Heat Vaporization at 30 °C (kJ/kg)	2431
Specific Heat of Cold Water (j/kg°C)	4184
Density (kg/m^3)	998

3.2 What's a Condenser ?

In systems involving heat transfer, a **condenser** is a **heat exchanger** used to condense a gaseous substance into a liquid state through cooling. In so doing, the latent heat is released by the substance and transferred to the surrounding environment. Condensers are used for efficient heat rejection in many industrial systems. Condensers can be made according to numerous designs, and come in many sizes ranging from rather small (hand-held) to very large (industrial-scale units used in plant processes). For example, a refrigerator uses a condenser to get rid of heat extracted from the interior of the unit to the outside air.

3.3 Hand Calculation

In the following section, we will explain the hand calculation with all needed details.
As you can see in **Figure** II.9, our system is a **Counter-flow** heat exchanger since the temperature of one of the fluids (steam) remains constant.
And here, why the temperature of the steam remains constant ?
The reason behind, is that the steam is changing it's phase from gas to liquid and we all know that matter state change is an **Isotherm Process**.

The temperature difference between the steam and the cooling water at the two ends of the condenser is

$$\Delta T_{LM1} = T_{h,in} - T_{c,out} = (30 - 22) = 8°C \quad \text{(II.3)}$$

$$\Delta T_{LM2} = T_{h,in} - T_{c,out} = (30 - 14) = 16°C \quad \text{(II.4)}$$

That is, the temperature difference between the two fluids varies from 8°C at one end to 16°C at the other. The proper average temperature difference be- tween the two fluids is the logarithmic mean temperature difference (not the arithmetic), which is determined from:

$$\Delta T_{LM} = \frac{\Delta T_1 - \Delta T_2}{\log(\frac{\Delta T_1}{\Delta T_2})} = \frac{8 - 16}{\log(\frac{8}{16})} = 11.5°C \quad \text{(II.5)}$$

As we can see in **Equation** (II.5), the ΔT_{LM} is less than $12°C$, so we can easily determine the **Heat Transfer rate** in our condenser using the expression below:

$$\dot{Q} = UA_s\Delta T_{LM} = (2100) * (45) * (11.5) = 1087\ kW \quad \text{(II.6)}$$

Where:

- U is the Overall heat coefficient
- A_s is the surface area of our condenser

That means the steam will lose heat at a rate of 1,087 kW as it flows through the condenser, and the cooling water will gain practically all of it, since the con- denser is well insulated.

The mass flow rate of the cooling water and the rate of the condensation of t steam are determined from this expression:

$$\dot{Q} = \dot{m}C_p(T_{out} - T_{in} = \dot{m}h_{fg} \tag{II.7}$$

So we can easily determine the **The mass flow rate of the cooling water** after simplifying this expression:

$$\dot{m}_{cooling\ water} = \frac{\dot{Q}}{C_p(T_{out} - T_{in})} \tag{II.8}$$

Where C_p is the **specific heat** of the cold water at $18°C$

So, we calculate $\dot{m}_{cooling\ water}$:

$$\dot{m}_{cooling\ water} = \frac{1.087}{4.184(22 - 14)} = 32.5\ kg/s \tag{II.9}$$

so, our target value for $\dot{m}_{steam}$ will be:

$$\dot{m}_{steam} = \frac{\dot{Q}}{h_{fg}} = \frac{1.087}{2431} = 0.45\ kg/s \tag{II.10}$$

What's the Heat Vaporization ?
The enthalpy of vaporization (symbol $\Delta Hvap$), also known as the (latent) heat of vaporization or heat of evaporation, is the amount of energy (enthalpy) that must be added to a liquid substance to transform a quantity of that substance into a gas. The enthalpy of vaporization is a function of the pressure at which that transformation takes place.
Therefore, we need to circulate about **72 kg** of cooling water for each 1 kg of steam condensing to remove the heat released during the condensation process.

Could we find approximately the same result with simulation ?

3.4 Aspen Hysys Simulation

3.4.1 1^{st} Method's Simulation

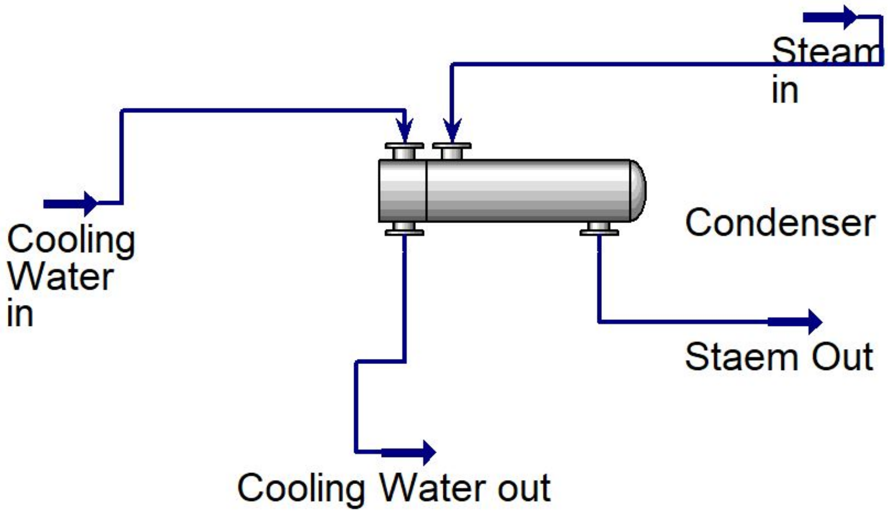


Figure II.10 – Flowsheet Case Design

Why i have called it a **First Method ?**
In this *Subsection*, i used the Classic **Heat Exchanger** option available in Aspen Hysys, which means that i have considered my **Condenser** as a classic Heat Exchanger *(because we can specify it as a **Cooler** option, which will be the topic of the next Subsection)*

Below, the Steps to follow for our simulation:

1. In **Component Lists** specify **Water** as your fluid.
2. for **Fluid Packages** you **Shloud** choose **ASME Steam** because here, we are using a steam and we should take into consideration the change of state of the steam (which is occurring at a constant temperature)
3. Now, go to **Simulation** and in your Model Palette, choose a **In Stream**, which i called it here **Cooling Water in** and we enter the specific Data.
   Note that the pressure we specified was of **1 barg** (2.013 relative bar), what means the 1 barg ? it's the **absolute bar** which is a pressure scale whose zero corresponds to perfect

vacuum and in french it's the **bar gauge** so we call it **barg** and we choose the barg scale because we want to indicate the absolute pressure so when using the steam which will change it's state, we get it's real temperature (exactly the true one) and we can't get it using the relative bar.

We should specify that the **Vapour phase fraction** is equal to zero. You can see **Figure** II.11 for DATA set.

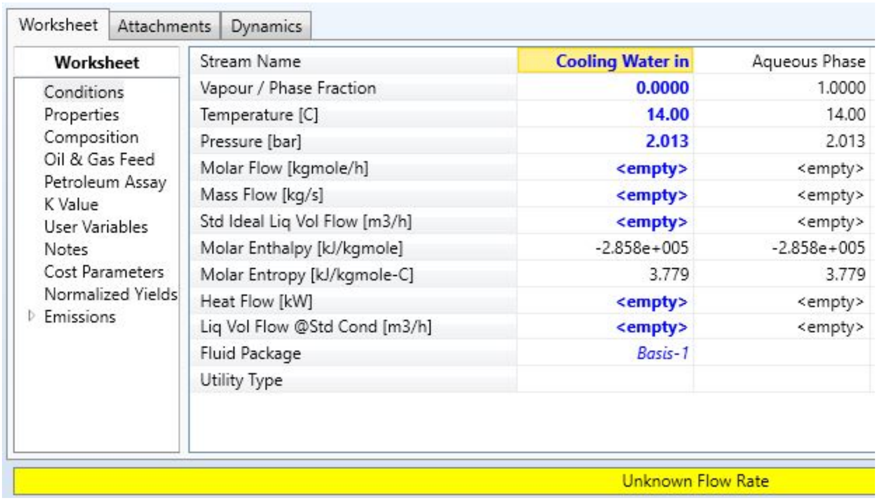


Figure II.11 – Inlet Cooling Water Design

4. Now, go to the Model Palette, and select your heat exchanger Icon, see **Figure** II.16

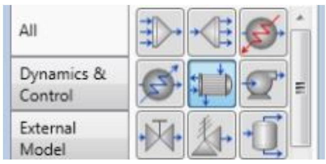


Figure II.12 – Heat exchanger Icon

5. Now, in the Interface of the Heat Exchanger, define your **Tube side Inlet** and **Outlet**, the outlet we called it **Cooling Water out**.

6. The next step is to **Rate** your exchanger, so go to **Rating** option and specify the **Heat Transfer Area Per Shell by modifying the Tube Dimension, the tube lentgh should be of 4.470 m** in order to get the Area of **45** m^2 so here we get an **experimental Area** of 44.49 m^2 which it almost the theoretical one. See **Figure** II.14

7. Now specify the **Overall Heat Area Coefficient UA**: By multiplying the **Overall Heat Coefficient** by the Area:

$$UA = U*A = 2100*45 = 94500W/°C = 94500J/s°C = \frac{94500*3600}{1000} = 3.402.10^5\ kJ/C.h \tag{II.11}$$

As we can see, the **Overall Coefficient U** we get is **2103** W/m^2K which is so close to the one given in the problem (2100).

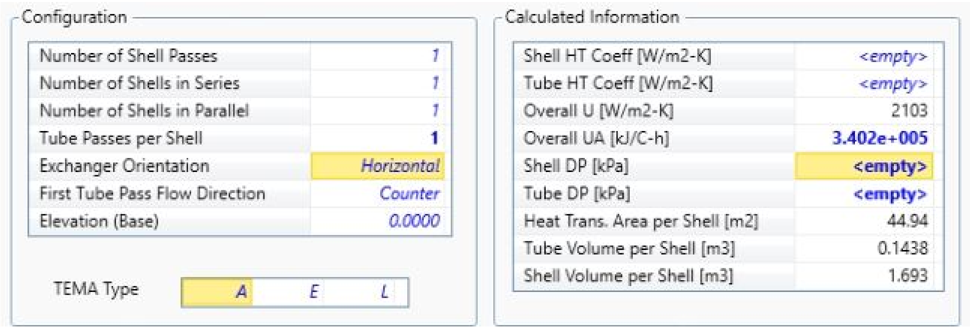


Figure II.13 – Rating the Exchanger

8. Now, we get back to the **Design** option, and we fill the **Shell side Inlet and Outlet** as **Steam in** and **Steam Out** respectively.

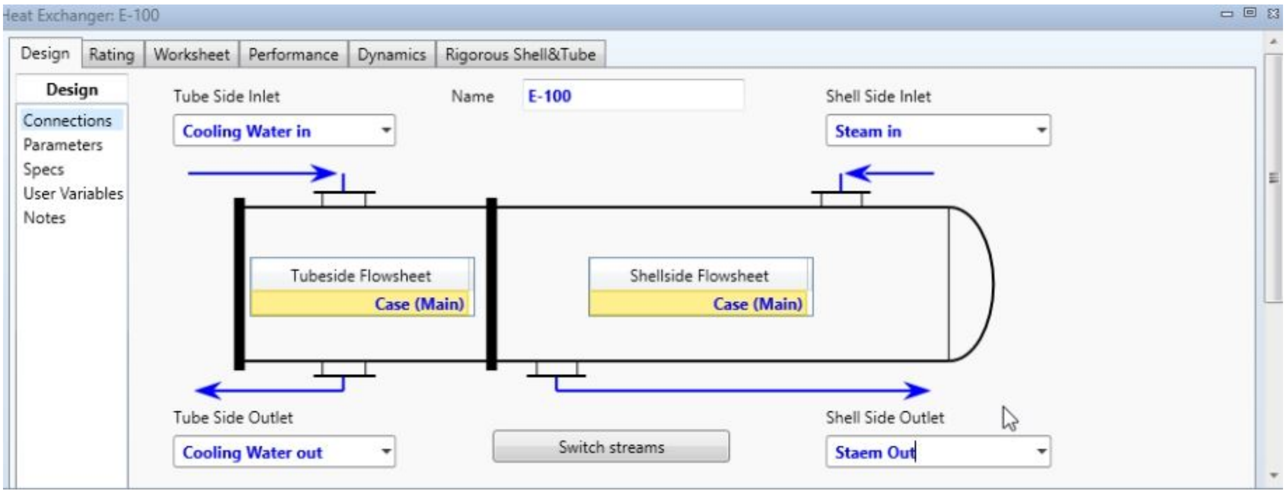
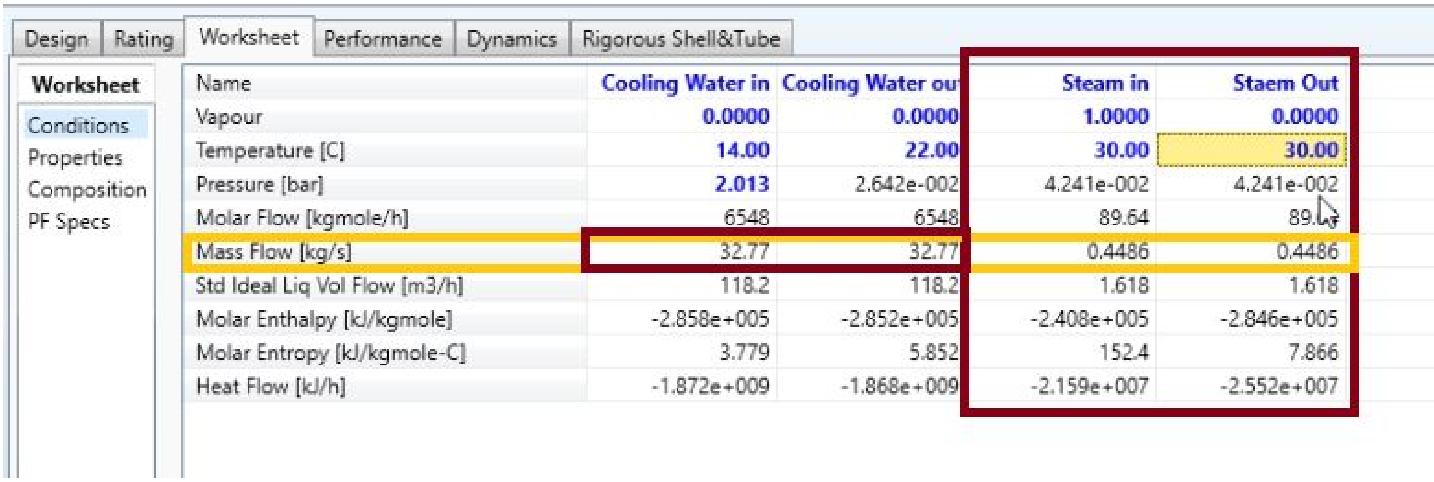


Figure II.14 – Rating the Exchanger

9. The next step consists of filling the **Worksheet** paper with information about the **Cooling water out**, **Steam in** and **Steam Out**.
Note That the Vapour fraction should be equal to "1" for either Steam in and Out Streams, also we should specify the Temperature which is constant and equal to $30°C$ and then Aspen will calculate the pressure as the Steam is condensing at $30°C$, means it is under vacuum. So we find it's pressure, which is the pressure of the steam condensation equal to $4.241.10^{-2}$ bar

10. Now, by just filling the **Vapour Fraction** of "0" (as the steam is already condensed, so it was transferred to a liquid) and the **temperature** of $30°C$, ASPEN will automatically calculate all needed DATA for the problem. See **Figure** II.15



Name	Cooling Water in	Cooling Water ou	Steam in	Staem Out
Vapour	0.0000	0.0000	1.0000	0.0000
Temperature [C]	14.00	22.00	30.00	30.00
Pressure [bar]	2.013	2.642e-002	4.241e-002	4.241e-002
Molar Flow [kgmole/h]	6548	6548	89.64	89.6
Mass Flow [kg/s]	32.77	32.77	0.4486	0.4486
Std Ideal Liq Vol Flow [m3/h]	118.2	118.2	1.618	1.618
Molar Enthalpy [kJ/kgmole]	-2.858e+005	-2.852e+005	-2.408e+005	-2.846e+005
Molar Entropy [kJ/kgmole-C]	3.779	5.852	152.4	7.866
Heat Flow [kJ/h]	-1.872e+009	-1.868e+009	-2.159e+007	-2.552e+007

Figure II.15 – Worksheet DATA for Steam In and Out

11. So as we can see, the **Mass Flow** of the **cooling water** and **Steam** were respectively **32.77 kg/s** and **0.4486 kg/s** which are almost the same of those found by Hand Calculation.

Table II.1 – Synthesis Table

Mass Flow (kg/s)	Hand Calculation	Simulation Calculation
Cooling Water	**32.5**	**32.77**
Steam	**0.45**	**0.4486**

Synthesis

Table III.1 indicates how the Simulation results are so close to the Hand calculated ones. We can, as a result, admit our simulation process and **accept** these values.

Are you ready to Compare this approach with the second method used in the simulation process ?

3.4.2 2^{nd} Method's Simulation

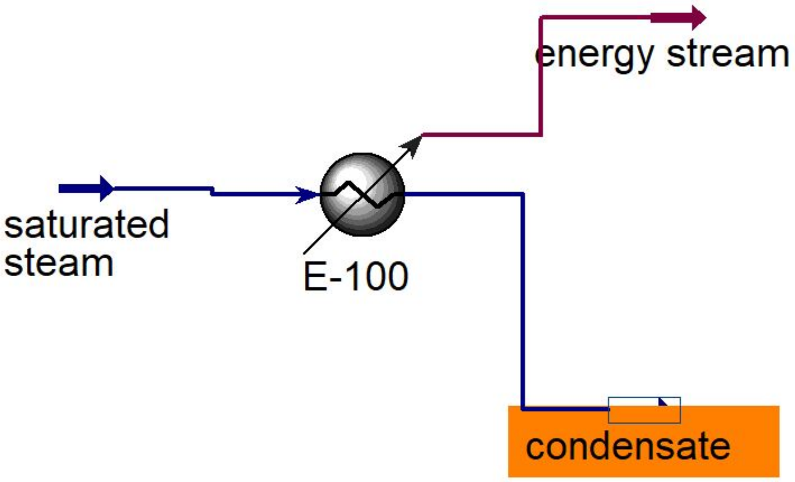


Figure II.16 – Flowsheet case

Now you should be able to understand why i have called it a second method, as you can see, in this method, i have used the **Cooler** Option in aspen instead of using the **Heat Exchanger** option and the reason behind is that our Steam is being **Condensed** so **Cooled**, so we can try to use the **Cooler** option and see if we will get the same result as the previous simulation method as well as the Hand calculation method.

Below the Steps to follow in order to succeed this simulation method

1. In **Component Lists** specify **Water** as your fluid.
2. for **Fluid Packages** you **Shloud** choose **ASME Steam** because here, we are using a steam and we should take into consideration the change of state of the steam (which is occurring at a constant temperature)
3. In the Model Palette, select The **Cooler** Icon, see **Figure** II.18

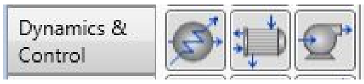


Figure II.17 – Cooler Icon

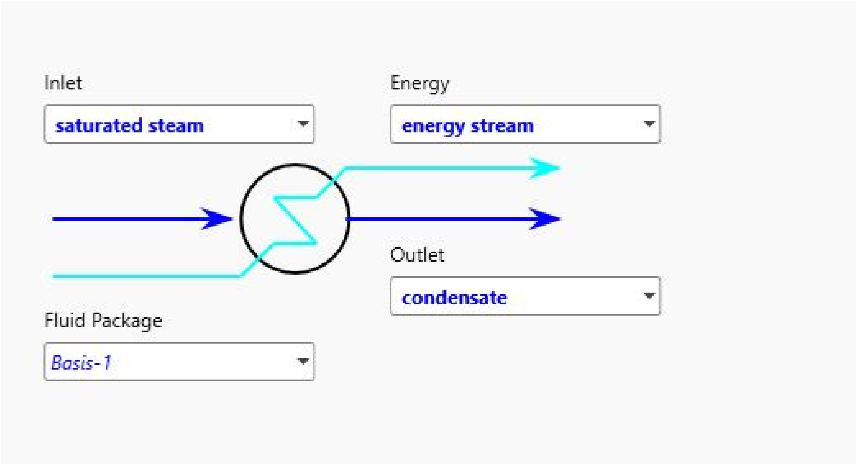


Figure II.18 – Cooler Design

4. Define your **Inlet**, **Outlet** and **Energy** Streams. Here i have called them respectively **Saturated Steam, Condensate and Energy Stream.**

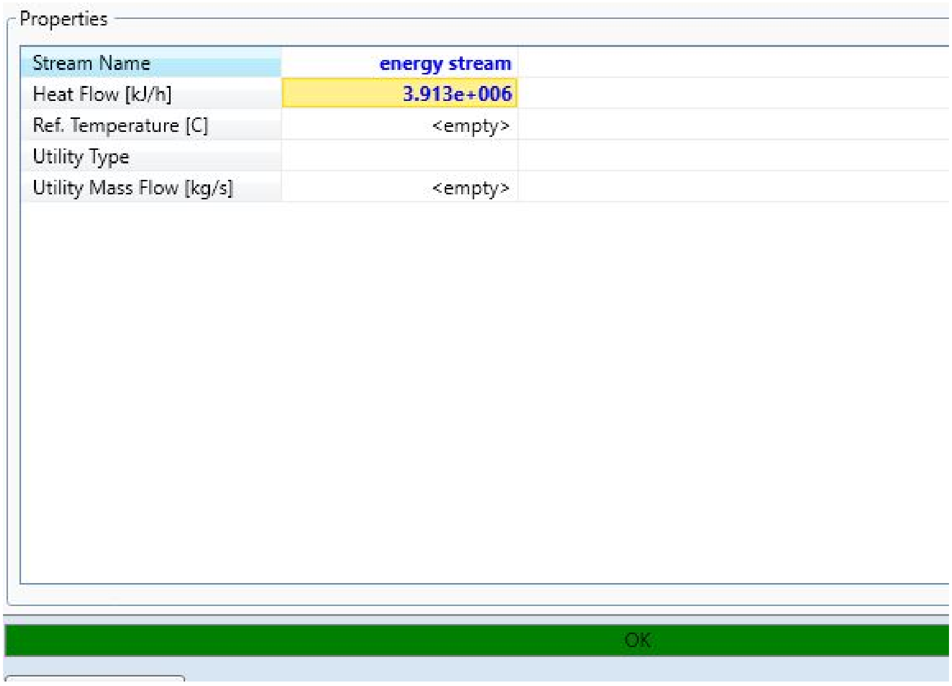
5. Now define your **Saturated steam** material, by entering a **Vapour Phase fraction** of "1" , a **Temperature** of 30°C and a **Composition**, Aspen will automatically calculate the pressure required as you can see in the **Figure** II.20

Stream Name	saturated steam	Vapour Phase	Aqueous Phase
Vapour / Phase Fraction	1.0000	1.0000	0.0000
Temperature [C]	30.00	30.00	30.00
Pressure [bar]	4.241e-002	4.241e-002	4.241e-002
Molar Flow [kgmole/h]	89.35	89.35	0.0000
Mass Flow [kg/s]	0.4471	0.4471	0.0000
Std Ideal Liq Vol Flow [m3/h]	1.613	1.613	0.0000
Molar Enthalpy [kJ/kgmole]	-2.408e+005	-2.408e+005	-2.846e+005
Molar Entropy [kJ/kgmole-C]	152.4	152.4	7.866
Heat Flow [kJ/h]	-2.152e+007	-2.152e+007	0.0000
Liq Vol Flow @Std Cond [m3/h]	1.611	1.611	0.0000
Fluid Package	Basis-1		
Utility Type			

Figure II.19 – Worsheet of Saturated steam

6. Now, the most **Important** step is to define your **Energy Stream**: to do, go to Energy stream arrow and you should enter the adequate value of **Heat Flow**, from where we get it ?

   You can check our **Hand Calculation** within the **Equation** (II.6) to find that our Heat flow was found to be: $\dot{Q} = 1087\ kW$ so it will be equal to $\dot{Q} = 3.913.10^6\ kJ/h$



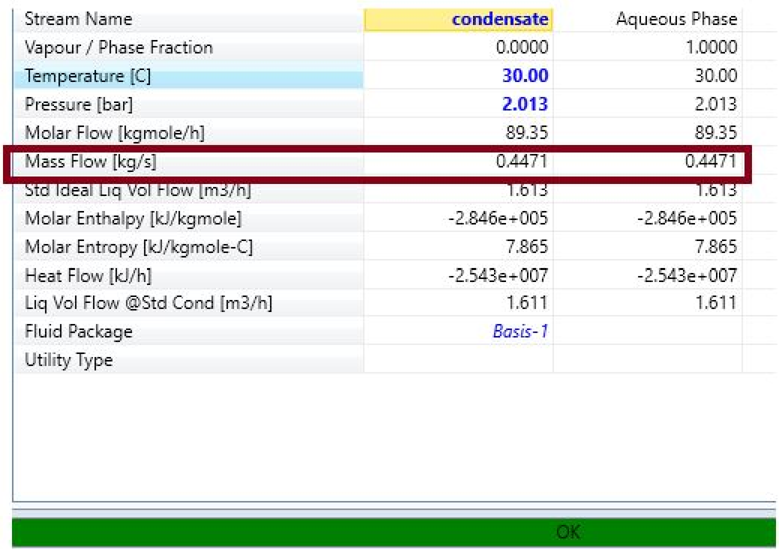
Properties

Stream Name	energy stream
Heat Flow [kJ/h]	3.913e+006
Ref. Temperature [C]	<empty>
Utility Type	
Utility Mass Flow [kg/s]	<empty>

OK

Figure II.20 – Properties of Energy stream

7. The Last step is to check our **Condensate** Stream and define the **Vapour Phase Fraction** as "0" (as it is Liquid now) and the **Temperature** of 30°C and now Aspen will calculate the **required Mass Flow**, as you can see in the **Figure** II.21 we get a **Mass Flow** of **0.4471 kg/s**.



Stream Name	condensate	Aqueous Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	30.00	30.00
Pressure [bar]	2.013	2.013
Molar Flow [kgmole/h]	89.35	89.35
Mass Flow [kg/s]	0.4471	0.4471
Std Ideal Liq Vol Flow [m3/h]	1.613	1.613
Molar Enthalpy [kJ/kgmole]	-2.846e+005	-2.846e+005
Molar Entropy [kJ/kgmole-C]	7.865	7.865
Heat Flow [kJ/h]	-2.543e+007	-2.543e+007
Liq Vol Flow @Std Cond [m3/h]	1.611	1.611
Fluid Package	Basis-1	
Utility Type		

OK

Figure II.21 – Material Stream Worksheet of Condensate

So, the result is approximately as the Hand calculated one, but we should **mention that this method is less precise than the previous one as we didn't introduce the Cooling Stream (Cold water) as it is an integrated Fluid in the Cooler (but it could be another fluid, not necessarily the water)**

4 Synthesis

The Table below summarises the **Hand Calculation Results** and Those found with **the two process Methods**

Table II.2 – Comparison Chart of Hand and Simulation Calculation

Mass Flow (kg/s)	Hand Calculation	Simulation Calculation 1	Simulation Calculation 2
Cooling Water	**32.5**	**32.77**	—
Steam	**0.45**	**0.4486**	**0.4471**

So as we have said previously, this little difference is due to the fact that the **Cooler** option does not include the Cooling Fluid such as water to choose it's Mass Flow rate.
Our Hand calculated results match very well with the ones obtained by simulation process, this difference is due to some parameters which are not specified in the problem DATA.
As a **conclusion**, we should be satisfied with these results as we are very close to the Theoretical ones.
(Even though we do not have some parameters like Pressure and Tube Shell Dimension, but with Surface Area, we can Specify them Approximately) .

Chapter III

Refrigeration Cycle

Contents

Introduction

This chapter will present The Technology of Refrigeration machine and the thermodynamic Concept behind it.

1 What's Refrigeration ?

The term refrigeration means cooling a space, substance or system to lower and/or maintain its temperature below the ambient one (while the removed heat is rejected at a higher temperature)[9]. In other words, refrigeration is artificial (human-made) cooling [9].
Energy in the form of heat is removed from a low-temperature reservoir and transferred to a high-temperature reservoir. The work of energy transfer is traditionally driven by mechanical means, but can also be driven by heat, magnetism, electricity, laser, or other means. Refrigeration has many applications, including household refrigerators, industrial freezers, cryogenics, and air conditioning. Heat pumps may use the heat output of the refrigeration process, and also may be designed to be reversible, but are otherwise similar to air conditioning units.
Refrigeration has had a large impact on industry, lifestyle, agriculture, and settlement patterns. The idea of preserving food dates back to at least the ancient Roman and Chinese empires. However, mechanical refrigeration technology has rapidly evolved in the last century, from ice harvesting to temperature-controlled rail cars. The introduction of refrigerated rail cars contributed to the westward expansion of the United States, allowing settlement in areas that were not on main transport channels such as rivers, harbors, or valley trails. Settlements were also developing in infertile parts of the country, filled with newly discovered natural resources.

2 Basic Fundamentals of refrigeration machines

We all know from experience that heat flows in the direction of decreasing temperature, that is, from high-temperature regions to low-temperature ones. This heat-transfer process occurs in nature without requiring any devices. The reverse process, however, cannot occur by itself. The transfer of heat from a low-temperature region to a high-temperature one requires special devices called **refrigerators** or **Refrigeration machines**.
Refrigerators are cyclic devices, and the working fluids used in the refrigeration cycles are called **refrigerants**.
Here is Figure III.12 explaining the mechanism with which a refrigerator functions.
Here Q_L is the magnitude of the heat removed from the refrigerated space at temperature T_L, Q_H is the magnitude of the heat rejected to the warm space at temperature T_H, and $W_{net,in}$

is the net work input to the refrigerator, note that Q_L and Q_H represent magnitudes and thus are positive quantities.

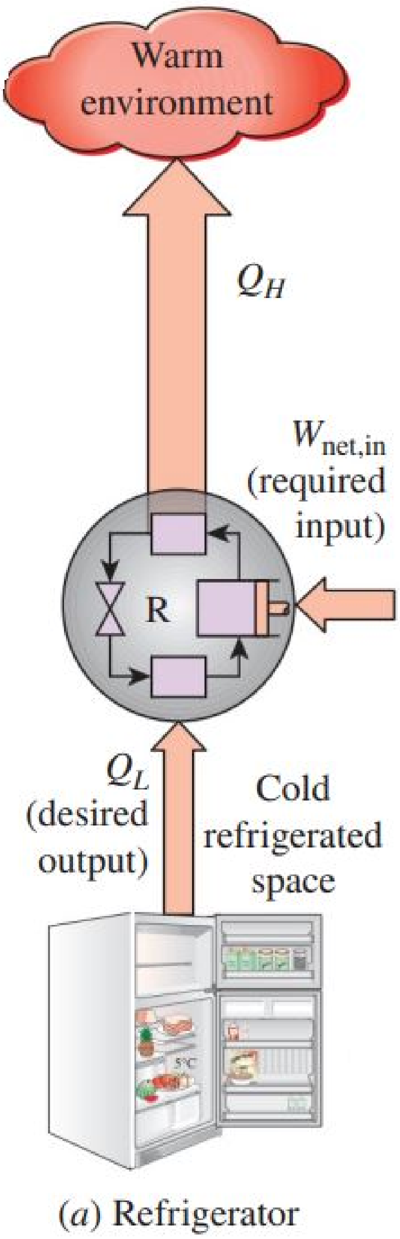


Figure III.1 – The Machanism of fucntion of a Refrigerating machine

2.1 What's the Thermodynamic ?

The thermodynamics is a branch of physics that deals with the dependence of physical properties of the body at the temperature , phenomena occur in which the heat exchanges , and transformation of energy between different forms. The study of ideal gases and that of thermal machines , which exchange energy with the outside in the form of work and heat , occupy a central place in thermodynamics.
Hot and cold notions have always existed. In 1780, **Pierre Simon de Laplace and Antoine Laurent de Lavoisier** wrote jointly [10] : "Whatever the cause which produces the sensation of heat, it is susceptible of increase and decrease, and, from this point of view, it may be subject to calculation. It does not seem that the ancients had the idea of measuring its relations, and it is only in the last century that one imagined means to achieve it.

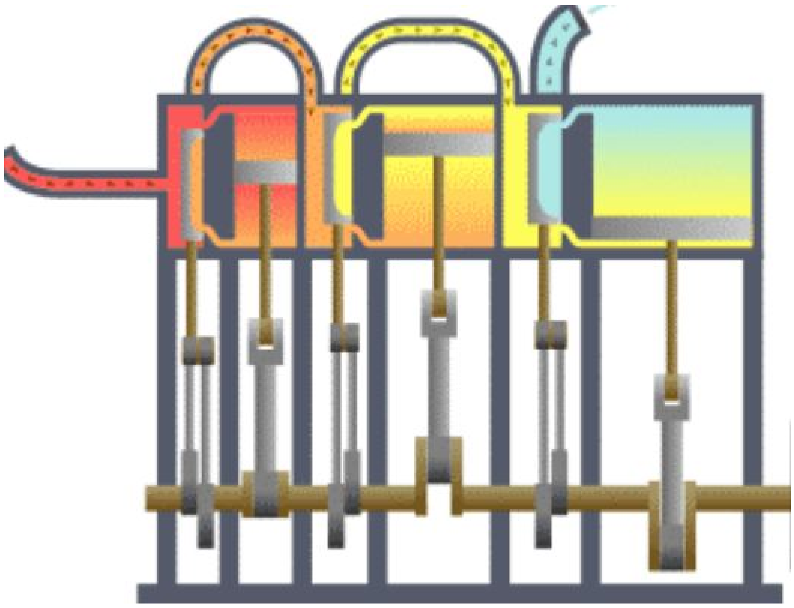


Figure III.2 – Typical thermal machine: heat moves from hot to cold and work is produced.

2.2 Thermodynamic Cycle

According to the second law of thermodynamics heat cannot spontaneously flow from a colder location to a hotter area; work is required to achieve this.
An air conditioner requires work to cool a living space, moving heat from the cooler interior (the heat source) to the warmer outdoors (the heat sink). Similarly, a refrigerator moves heat from inside the cold icebox (the heat source) to the warmer room-temperature air of the kitchen (the heat sink). The operating principle of ideal heat engine was described mathematically using

Carnot cycle by **Sadi Carnot** in 1824. An ideal refrigeration or a heat pump system can be thought of as an ideal heat engine that is operating in a reverse Carnot cycle.
We have:

- **Vapor-compression cycle**: The vapor-compression cycle is used by many refrigeration, air conditioning and other cooling applications and also within heat pump for heating applications.
- **Vapor absorption cycle**: In the early years of the twentieth century, the vapor absorption cycle using water-ammonia systems was popular and widely used but, after the development of the vapor compression cycle, it lost much of its importance because of its low coefficient of performance (about one fifth of that of the vapor compression cycle)
- **Gas cycle**: When the working fluid is a gas that is compressed and expanded but does not change phase, the refrigeration cycle is called a gas cycle. Air is most often this working fluid. As there is no condensation and evaporation intended in a gas cycle, components corresponding to the condenser and evaporator in a vapor compression cycle are the hot and cold gas-to-gas heat exchangers.
- **Stirling engine Cycle**: **The Stirling cycle** heat engine can be driven in reverse, using a mechanical energy input to drive heat transfer in a reversed direction. There are several design configurations for such devices that can be built. Several such setups require rotary or sliding seals, which can introduce difficult tradeoffs between frictional losses and refrigerant leakage.
- **Reversed Carnot cycle**: The Carnot cycle is a reversible cycle so the four processes that comprise it, two isothermal and two isentropic, can also be reversed. When a Carnot cycle runs reversely, it is called a reversed Carnot cycle. A refrigerator or heat pump that acts on the reversed Carnot cycle is called a Carnot refrigerator or Carnot heat pump respectively.

2.3 Coefficient of Performance

The efficiency of a refrigerator or heat pump is given by a parameter called the coefficient of performance (COP).
The equation is:

$$COP = \frac{Q}{W} \tag{III.1}$$

Where

- Q is the useful heat supplied or removed by the considered system.
- w is the work required by the considered system.

The Detailed COP of a refrigerator is given by the following equation:

$$COP_R = \frac{DesiredOutput}{RequiredInput} = \frac{CoolingEffect}{WorkInput} = \frac{Q_L}{W_{net,in}} \tag{III.2}$$

For **Carnot refrigerators**, **COP** can be expressed in terms of temperatures:

$$COP_{R,Carnot} = \frac{T_L}{T_H - T_L} = \frac{1}{(\frac{T_H}{T_L}) - 1} \tag{III.3}$$

2.4 Compressor

A mechanical compressor is a mechanical device intended to increase the pressure of a gas and therefore its energy .
There are also compressors without any mechanical component these are thermocompressors[11], more commonly called ejectors.

Figure III.3 – Refrigerator Compressor

2.5 Condenser

A condenser is a heat exchanger used to condense a gaseous substance into a liquid state through cooling. In so doing, the latent heat is released by the substance and transferred to the surrounding environment. Condensers are used for efficient heat rejection in many industrial systems.

Figure III.4 – Condenser Coil of a refrigerator

2.6 Expansion Valve

An expansion valve is a device in steam engine valve gear that improves engine efficiency. It operates by closing off the supply of steam early, before the piston has travelled through its full stroke. This cut-off allows the steam to then expand within the cylinder[12]

2.7 Evaporator

An evaporator is a device in a process used to turn the liquid form of a chemical substance such as water into its gaseous-form/vapor. The liquid is evaporated, or vaporized, into a gas form of the targeted substance in that process.

Figure III.5 – Expansion Valve of Refrigheration machines

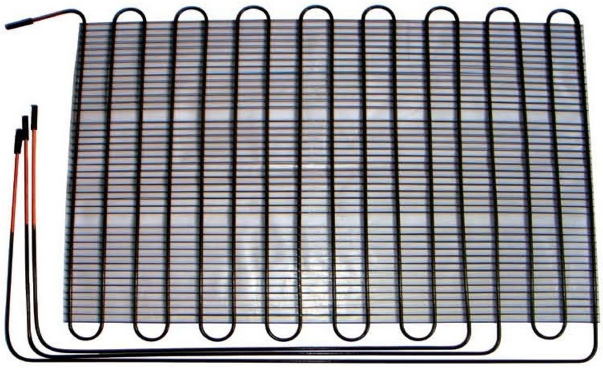


Figure III.6 – Refrigerator Evaporator

3 Study of The Actual Vapor-Compression Refrigeration Cycle

3.1 Introduction

Refrigerant **-134a** enters the compressor of a refrigerator as superheated vapor at 0.14 MPa and $-10°C$ at a rate of 0.05 kg/s and leaves at 0.8 MPa and 50°C. The refrig- erant is cooled in the condenser to 26°C and 0.72 MPa and is throttled to 0.15 MPa. Disregarding any heat transfer and pressure drops in the connecting lines between the components.
We should determine the rate of heat removal from the refrigerated space and the power input to the compressor, the isentropic efficiency of the compressor and finally the coefficient of performance of the refrigerator

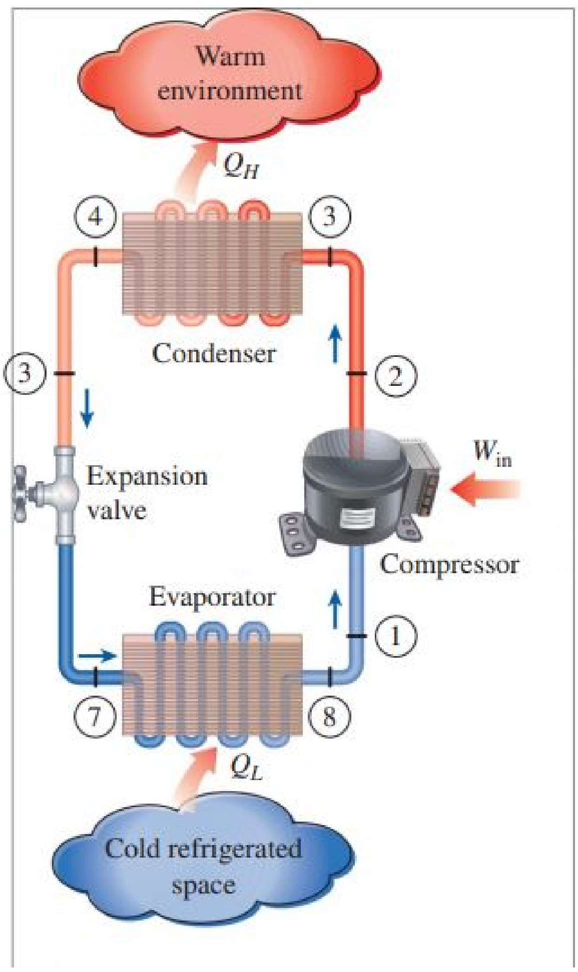


Figure III.7 – Schematic representation of the refrigeration machine

3.2 Detailed Hand Calculation

First of all, what's the **Fluid 134a ?**
The 1,1,1,2-tetrafluoroethane is a hydrocarbon halogenated empirical formula $C_2H_2F_4$. It is mainly used as **a refrigerant** under the name **R-134a or HFC-134a**.
Composed of the class of hydrofluorocarbons (HFCs), it has no impact on the ozone layer (ODP = 0), and thus has been designated to replace the various CFCs (in particular dichlorodifluoromethane R-12) in the cooling system, but it contributes greatly to the greenhouse effect and its content in the air has been increasing steadily since around 1990.

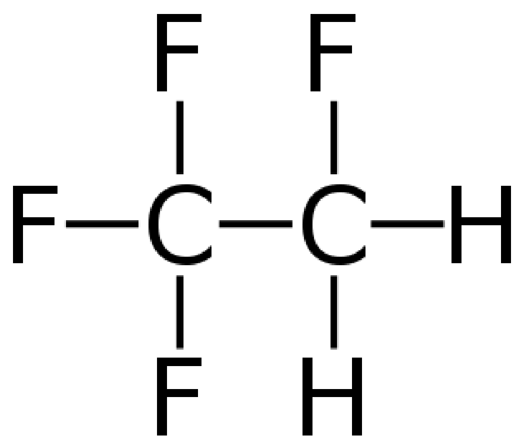


Figure III.8 – A depiction of the chemical structure of 1,1,1,2-Tetrafluoroethane

Hypotheses and Assumptions:
We admit that we have a steady operating conditions and the Kinetic and potential energy changes are negligible.
In order to understand the correct principle of the refrigeration cycle, below the **Temperature-Entropy: T-s** diagram of the refrigeration cycle.
We note that the refrigerant leaves the condenser as a compressed liquid and enters the compressor as superheated vapor. The enthalpies of the refrigerant at various states are determined from the refrigerant tables to be:
$P_1 = 0.14\ MPa, T_1 = -10°C, h_1 = 246.37kj/kg$
$P_2 = 0.8\ MPa, T_2 = 50°C, h_2 = 286.71kj/kg$
$P_3 = 0.72\ MPa, T_3 = 26°C, h_3 = 87.83kj/kg$
$h_4 = h_3 = 246.37kj/kg$

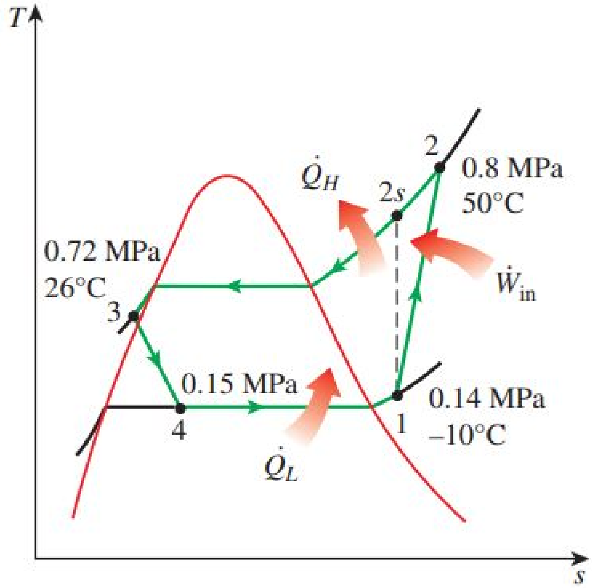


Figure III.9 – T-S Diagram for the 134a refrigeration Cycle

1. **The rate of heat removal from the refrigerated space and the power input to the compressor are determined from their definitions:**

$$Q_L = \dot{m}(h_1 - h_4) = 0.05(246.37 - 87.83) = 7.93\ kW \tag{III.4}$$

and

$$W_{in} = \dot{m}(h_2 - h_1) = 0.05(286.71 - 246.37) = 2.02\ kW \tag{III.5}$$

2. The isentropic efficiency of the compressor is determined from:

$$\eta_r = \frac{h_{2s} - h_1}{h_2 - h_1} \tag{III.6}$$

where the enthalpy at state 2s ($P_{2s} = 0.8MPa, \quad s_{2s} = s_1 = 0.9724kJ/kgK$) is $284.20kJ/kg$. Thus,

$$\eta_r = \frac{284.20 - 246.37}{286.71 - 246.37} = 0.938 : 93.8\% \tag{III.7}$$

3. (c) The coefficient of performance of the refrigerator is:

$$COP_R = \frac{\dot{Q}_L}{\dot{W}_{in}} = \frac{7.93}{2.02} = 3.93 \tag{III.8}$$

3.3 Synthesis

Below we summarize the most important Hand calculated results that we need in our simulation process.

Table III.1 – Hand Calculated synthesis Table

$\dot{Q}_L$ (kW)	W_{in} (kW)
7.93	**2.02**

3.4 Simulation process

3.4.1 How should we choose the thermodynamic model and package for Aspen ?

To calculate the rate of heat removal from **the refrigerated space** $\dot{Q}_L$ and **the power input to the compressor** W_{in} for different conditions in process simulation Aspen Plus, there are thermodynamic models, model parameters and calculation procedures available.
There are two common methods for representing the fugacity coefficients from the phase equilibrium relationship in terms of measurable state variables, **the equation of state method** and the **activity coefficient method**

- **Equation of state methods** use the various equations of state from chemical engineering thermodynamics to calculate the equilibrium conditions. The two most familiar are **PR (Peng and Robinson, 1976)** and **SRK** or **Soave-Redlich-Kwong (Soave, 1972)**. Both of them are cubic equations of state and they only need **critical properties and ideal gas enthalpies for each component** to calculate all the necessary thermodynamic properties for equilibrium calculations.

- **An activity coefficient method** is a more empirical approach to calculate the equilibrium. This method uses various relationships to calculate the liquid phase activity coefficient and then the fugacity coefficient. A common activity model is **NRTL or Non-Random Two Liquid (Renon and Prausnitz, 1968)**. In Aspen Plus ideal gas enthalpy and heat of vaporization correlations are used to calculate enthalpies. The **NRTL model** is the same in Aspen HYSYS and Aspen Plus as in the original paper. The results from an activity model are dependent on the parameter values for the components and enthalpy correlations. These parameter values may be different in different program versions.

But which model to choose for the R134a Fluid ?

First of all, our Refrigerant fluid which is the **1,1,2-Tetrafluoroethane** is a **non-polar** substance and if we consult **Aspen Plus** and see the Physical Properties of this fluid, we find that it's **Critical Temperature** is $101.03°C$ and during our process, we are operating under this critical temperature, so we should use **an equation of state method**, we can use **SRK** and **Wilson**, so during our process simulation, we will use the **Wilson and NRK Thermodynamic package** and we will compare the results as these two packages are the most accurate ones to use.

Problem Presentation

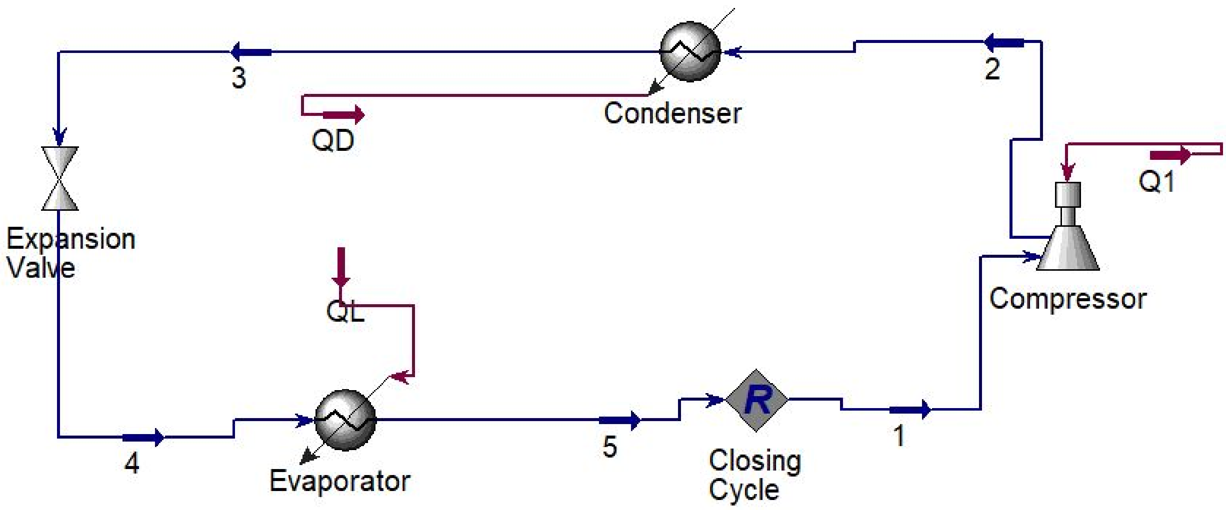


Figure III.10 – Process Flowsheet

For our process simulation, we are going to explain with details all the steps to follow:

- First Step consists of selecting our substance from the component list which is **1,1,1,2-TetraFluoroethane** then select the 1^{st} Fluid package which is **SRK** thermodynamic package, then we will reevaluate the results considering the **Wilson** thermodynamic package.
- After proceeding to the **Simulation Sheet**, into the model palette, select the **Compressor** tool then define the **Inlet Flow** according to our case study.
- Now, proceed to the compressor parameters and select the right **Delta P** which is the pressure drop as $0.66\ MPa$ and as a result, Aspen will automatically design the **Outlet**

Stream Name	1	Vapour Phase
Vapour / Phase Fraction	1.0000	1.0000
Temperature [C]	-10.22	-10.22
Pressure [MPa]	0.1400	0.1400
Molar Flow [kgmole/h]	1.764	1.764
Mass Flow [kg/s]	5.000e-002	5.000e-002
Std Ideal Liq Vol Flow [m3/h]	0.1449	0.1449
Molar Enthalpy [kJ/kgmole]	-8.987e+005	-8.987e+005
Molar Entropy [kJ/kgmole-C]	234.4	234.4
Heat Flow [kJ/s]	-440.4	-440.4
Liq Vol Flow @Std Cond [m3/h]	0.1455	0.1455
Fluid Package	Basis-1	
Utility Type		

OK

Figure III.11 – Compressor Inlet Stream

Stream "2" and by just selecting the outlet stream, you can see that the **Outlet Temperature** is **54,59** $°C$, theoretically it is $50°C$ as mentioned in the problem Data. This little difference is due to the limitation of the thermodynamic package (which is by the way, the most accurate thermodynamic model).

- Now, from the model palette, select the **Cooler** tool which will be equivalent the **Condenser** device. We should select the Compressor Outlet Stream as the **Cooler Inlet stream**. Next Step is to define your **Outlet and Energy stream** (Q_D)

- Select the Parameters of your cooler: **Pressure Drop** is estimated to be **0.08 MPa** (which was calculated from the pressure difference of Inlet and Outlet Pressure), Select **Delta T** as **-33** $°C$ and so the **Duty** as well as **the outlet stream** will be automatically calculated by Aspen.
  The Temperature of **Outlet Condenser stream** was found to be **26.18** $°C$ which is almost the one given in the problem DATA (26 $°c$)

- Now, select the **Expansion Valve** from the Model Palette and define the **Condenser Outlet Stream "3" as a valve Inlet Stream**, define the Valve Outlet Stream as "4"

- Now, we should size the expansion valve, so go to parameters and define your **Delta P** as 0.57 MPa **Figure** III.14

Stream Name	3	Liquid Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	26.18	26.18
Pressure [MPa]	0.7200	0.7200
Molar Flow [kgmole/h]	1.764	1.764
Mass Flow [kg/s]	5.000e-002	5.000e-002
Std Ideal Liq Vol Flow [m3/h]	0.1449	0.1449
Molar Enthalpy [kJ/kgmole]	-9.153e+005	-9.153e+005
Molar Entropy [kJ/kgmole-C]	129.0	129.0
Heat Flow [kJ/s]	-448.5	-448.5
Liq Vol Flow @Std Cond [m3/h]	0.1455	0.1455
Fluid Package	Basis-1	
Utility Type		

OK

Figure III.12 – Condenser Outlet Stream

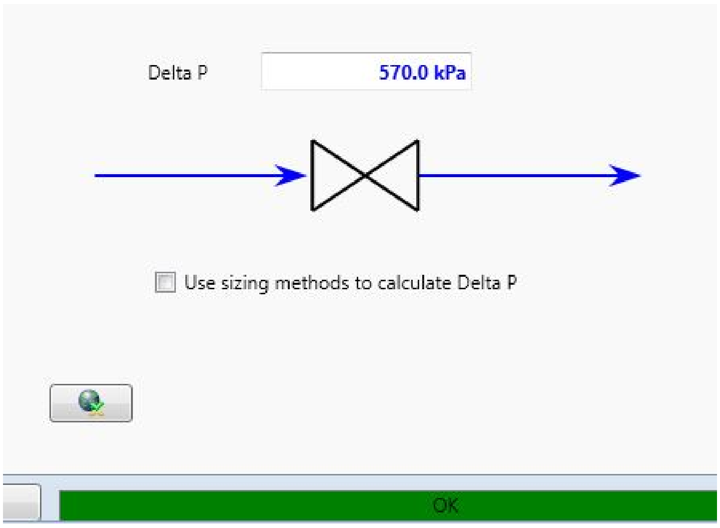


Figure III.13 – Pressure Drop in the Expansion valve

- The Last Device we should add the this cycle is for sure the **Evaporator**, in Aspen it is defined as a **Heater**, so select the **heater** from the model palette and define it's Inlet Stream as the Outlet stream of the expansion valve. Define also the **Outlet and Energy stream**

- As usual, we are going to define the parameters of the Evaporator:
  Pressure drop is estimated to be **0.01 MPa** (0.15MPa - 0.14MPa) and a **temperature**

difference of **07** $°C$ *(as we desire an Outlet temperature of the evaporator to be the same as the Compressor Inlet Temperature).*

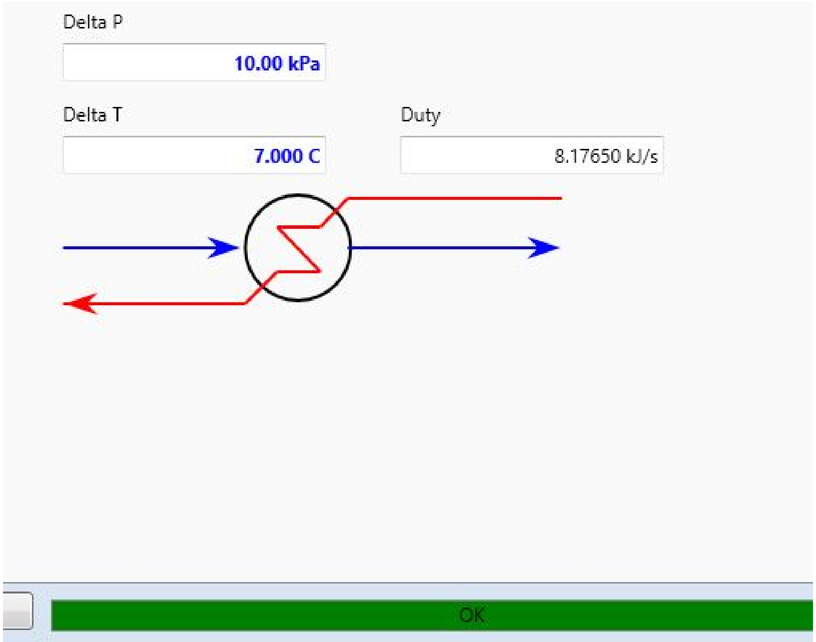


Figure III.14 – Pressure Drop in the Expansion valve

- **NOTE** that due to the package limitation and the simulation condition, the Evaporator Inlet Temperature was founded to be **-10.08** $°C$ and the one mentioned in the problem was -10 $°C$ and this is acceptable as we are manipulating as a simulation scenario, and that Aspen did not consider all the emitted hypotheses we have mentioned in the **Hand Calculation Section** See **Figure** III.15
- Now, in order to **Close the cycle**, we can use the utility **Recycle: RCY** which you find it in the model palette. We called it "Closing Cycle".
- So, now it's time to evaluate the Simulation process results, to do, we select the evaporator (Heater) **Energy Stream Heat Transfer** or also called the **Rate of heat removal from the refrigerated space**, so we find (see **Figure** III.16 and III.17)

$$\dot{Q}_L = 7.958\ kW \tag{III.9}$$

and **the power input to the compressor** is

$$\dot{W}_{in} = 2.543\ kW \tag{III.10}$$

Stream Name	5	Vapour Phase
Vapour / Phase Fraction	1.0000	1.0000
Temperature [C]	-10.08	-10.08
Pressure [MPa]	0.1400	0.1400
Molar Flow [kgmole/h]	1.764	1.764
Mass Flow [kg/s]	5.000e-002	5.000e-002
Std Ideal Liq Vol Flow [m3/h]	0.1449	0.1449
Molar Enthalpy [kJ/kgmole]	-8.989e+005	-8.989e+005
Molar Entropy [kJ/kgmole-C]	195.5	195.5
Heat Flow [kJ/s]	-440.5	-440.5
Liq Vol Flow @Std Cond [m3/h]	0.1455	0.1455
Fluid Package	Basis-1	
Utility Type		

OK

Figure III.15 – Evaporator Material Stream with conformity to the Inlet Condition of the Compressor

QL		
Heat Flow	7.958	kJ/s

Figure III.16 – Evaporator Energy Stream Heat Transfer

Compressor		
Feed Pressure	0.1400	MPa
Product Pressure	0.8000	MPa
Molar Flow	1.764	kgmole/h
Energy	2.532	kJ/s

Figure III.17 – Compressor Energy Input stream

We repeat the Simulation process using the Wilson package instead of SRK results will be reported in the next section.

3.5 Synthesis

Here we are summarizing the Hand calculation and Process simulation results in this table: We mean by:

- **ESHT**: Energy Stream Heat Transfer
- **PIC** : Power Input Compressor

Table III.2 – Comparison Chart of Hand and Simulation Calculation for the refrigeration cycle

	Hand Calculation	Simulation Calculation **SRK**	Simulation Calculation **Wilson**
ESHT (kW)	**7.93**	**7.958**	**8.1**
PIC (kW)	**2.02**	**2.543**	**2.723**

4 Conclusion

From the results reported in **Table** III.2, we can see that the simulation process gave us a satisfying results. They are close to the Hand calculated ones.
But we can detect a slight difference between **SRK and Wilson** packages results and it's completely a predictable behaviour as there is always some limitations into the fluid packages (because we are changing the state of our fluid).
From this comparison, we can adopt the **SRK** Simulation results as it shows the most accurate and suitable results comparing to the Hand calculation estimation.

Conclusion

- So, comparing results obtained with Hand calculation using Excel and those with Simulation using Aspen, we can say that we have almost the same results (near measuring errors) with the **Equivalent Lengths** Method **but it's a more satisfying result** using the **Colebrook** method when **we take into consideration all the present singularities in the pipe** and thus it's a **satisfying simulation result.**
  What we should say as a conclusion is that when we use the correct **Singularities** the results is much more **satisfying** than those obtained when we consider only an approximated Singularity length using the Equivalent Length method.
  We learned how to size a pipeline taking into consideration all variables needed.
  The importance of manual developing calculation is to ensure that we know the basics and principles of chemical Engineering because Aspen will not function correctly if we are not understanding what we should do and what we should expect.

- In the Heat Exchangers Chapter, as you can see, we detailed our Hand Calculation process, we explained the theory of Heat Transfer and the types of heat exchanger we can find for industrial use.
  It's very important to understand the Heat Transfers laws and to be able to apply it for any heat device.
  We detailed also the simulation process using **Aspen** and it's not only this, but we developed two methods for numerical resolution. By understanding the theory and Hand calculation, you will be able to understand the simulation process as it requires a lot of theoretical mastery. You can see that the results we got from simulation process are so satisfying comparing to the Hand Calculated ones. There is always a little difference, and this is due to the pressure, Tube diameters (Internal and Outside) which are not well specified is the problem, so it's our duty to **size** and this is the Engineering task.

- With the Refrigeration cycle problem, we are facing two issues in order to succeed the case study, we should first study which Thermodynamic model we will consider during the process, if it is an **equation of state** or an **activity coefficient method**, we should study the limitations of packages in the same category and choose the most suitable one that satisfies our theoretical results, but bear in mind that every package has it's own limitations and we can not have all the problem parameters close to the hand calculation results, but depending on which unity we want to value, we can make our choice of the package and the most accurate method to do this is by doing **experiments**, which means by doing many process simulation scenarios.

Appendix

1 Equivalence of pressure drops in straight pipe lengths

We Used this Chart to determine the equivalent lengths for the 45 °Elbows and the Globe valve fully open.

The red segment is referring to the 45 °elbow and the orange segment is referring to the Globe valve equivalent length.

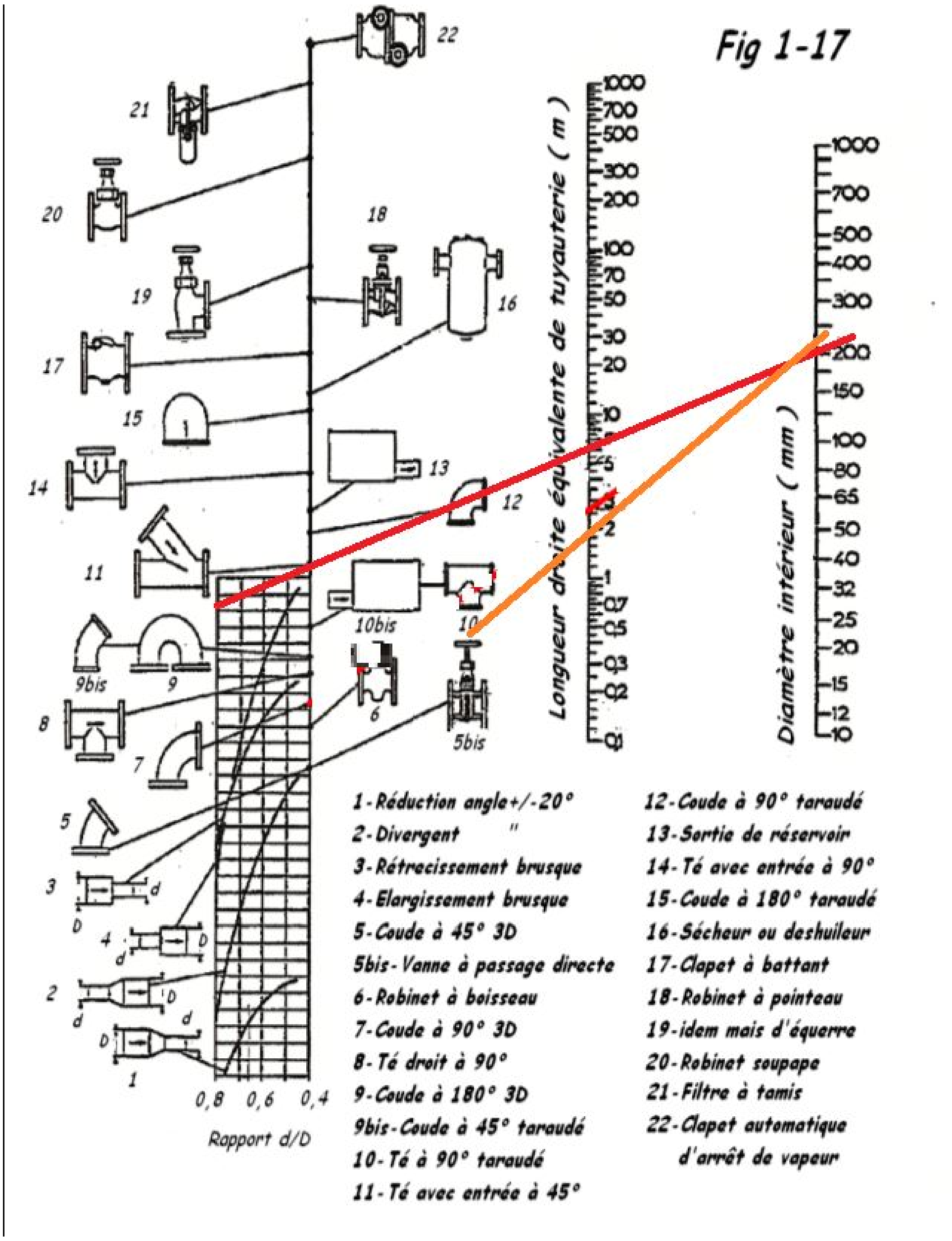


Figure 18 – Equivalence of pressure drops in straight pipe lengths Chart

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> My Congratulations on this work !
>
> - Dr. Sami ABID

AYMEN LABIDI

Is a chemist and a simulator pilot.
Born in Tunisia, he was educated at Hay El Ryadh School, El Rachidia College and Mourouj IV Hight School.
He studied at the National Intsitute of Applied Science and Technology INSAT.
Glider Manager for Aerobotix-INSAT and an aeronautical consultant for the FTAA, he gives onlines course session about the principle of flight and it's aerodynamic aspects.
LABIDI is the author of the Book "Quick Reference Handbook of Chemistry" for the beginners in the chemistry Field.
He frequently gives scientific information about chemistry and it's beauty.

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