ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL

COMPUTER-AIDED EXERGY AND ENERGY ANALYSIS OF THE VACUUM DISTILLATION UNIT

M.Sc. THESIS

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Thesis Advisor: Prof. Dr. Serdar YAMAN

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ISTANBUL TEKNİK ÜNİVERSİTESİ ★ LİSANSÜSTÜ EĞİTİM ENSTİTÜSÜ

VAKUM DİSTİLASYON ÜNİTESİNİN BİLGİSAYAR DESTEKLİ EKSERJİ VE ENERJİ ANALİZİ

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Sena KURBAN, a M.Sc. student of ITU Graduate School student ID 506181025, successfully defended the thesis entitled “COMPUTER-AIDED EXERGY AND ENERGY ANALYSIS OF THE VACUUM DISTILLATION UNIT”, which she prepared after fulfilling the requirements specified in the associated legislations, before the jury whose signatures are below.

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To my dear and pretty family,

FOREWORD

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Sena KURBAN
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ABBREVIATIONS

ADU	**:** Atmospheric Distillation Unit
ANN	**:** Artificial Neural Network
AR	**:** Atmospheric Residue
ASPEN	**:** Advanced System for Process Engineering
ASTM	**:** American Society for Testing and Materials
BANN	**:** Bootstrap Aggregated Neural Network
DOF	**:** Degrees of Freedom
EOS	**:** Equation of State
FBNN	**:** Feedback Neural Network
FFNN	**:** Feedforward Neural Network
FLT	**:** First Law of Thermodynamics
GA	**:** Generic Algorithm
HEN	**:** Heat Exchanger Network
HSO	**:** Heavy Slop Oil
HVGO	**:** Heavy Vacuum Gas Oil
IEA	**:** International Energy Agency
KNN	**:** K Nearest Neighbors
LMTD	**:** Logarithmic Mean Temperature Difference
LVGO	**:** Light Vacuum Gas Oil
MHVGO	**:** Medium and Heavy Vacuum Gas Oil
ML	**:** Machine Learning
MSE	**:** Mean Squared Error
MVGO	**:** Medium Vacuum Gas Oil
PA	**:** Pump Around
PFD	**:** Process Flow Diagram
PR	**:** Peng Robinson
RF	**:** Random Forest
RL	**:** Reinforcement Learning
RMS	**:** Root Mean Square
SL	**:** Supervised Learning

SLT : Second Law of Thermodynamics
SSL : Semi Supervised Learning
TBP : True Boiling Point
UL : Unsupervised Learning
VDU : Vacuum Distillation Unit
VGO : Vacuum Gas Oil
VR : Vacuum Residue

SYMBOLS

C	: Carbon
C	: Column
°C	: Degree Celsius
cv	: Control Volume
E	: Heat Transfer Equipment
$\dot{E}_e$	: Exit Energy Rate
$\dot{E}_i$	: Inlet Energy Rate
Ex	: Exergy Rate
ex	: Specific Exergy
Ex_{cold}	: Cold Stream Exergy Rate
$\dot{E}x_e$, $\dot{E}x_o$	: Exit or Outlet Exergy Rate
$\dot{E}x_i$	: Inlet Exergy Rate
$Ex_{flow,ph}$	: Physical Flow Exergy Rate
Ex_{flow}	: Flow Exergy Rate
Ex_{hot}	: Hot Stream Exergy Rate
ex_i^{ch}	: Specific Chemical Exergy
Ex_{in}	: Inlet Exergy Rate
Ex_{kin}	: Kinetic Exergy Rate
ex_{mix}^{ch}	: Mixture Specific Chemical Exergy
$Ex_{nonflow}$	: Nonflow Exergy Rate
Ex_o	: Chemical Exergy Rate
Ex_{out}	: Outlet Exergy Rate
Ex_{ph}	: Physical Exergy Rate
Ex_{pot}	: Potential Exergy Rate
Ex_Q	: Heat Exergy Rate
F	: Furnace
f(X)	: Aggregated Neural Network Forecaster
G	: Pump
g	: Gravity Acceleration

H : Enthalpy

h : Hour

h : Specific Enthalpy

H_{in} : Inlet Enthalpy

H_0 : Reference Enthalpy

h_0 : Reference Specific Enthalpy

H_{out} : Outlet Enthalpy

H_2 : Hydrogen

H_2O : Water

I : Irreversibility

i, f : Initial and Final Status

i, j : Species

$\dot{I}_{cv}$: Irreversible Exergy Loss of a Control Volume

in : Inlet or Input

K : Kelvin

kin : Kinetic

kj : Kilojoule

kPa : Kilopascal

LHV_i : Lower Heating Value

$\dot{m}_e$: Exit Mass Flow Rate

$\dot{m}_i$: Inlet Mass Flow Rate

mix : Mixture

n : Neural Networks Number

N_i : Moles Number

N_2 : Nitrogen

out : Outlet or Output

O_2 : Oxygen

P : Pressure

P_0 : Reference Pressure

ph : Physical

pot : Potential

Q : Heat Transfer Interaction

$\dot{Q}$: Heat Transfer Rate

$\dot{Q}_{cv}$: Heat Rate into Control Volume

R : Molar Gas Constant

$\mathbf{R^2}$	: Coefficient of Determination
rev	: Reversible
S	: Entropy
s	: Second
s	: Specific Entropy
S	: Sulfur
SG	: Specific Gravity
$\mathbf{S_{gen}}$	: Entropy Generation
$\mathbf{S_0}$	: Reference Entropy
$\mathbf{s_0}$	: Reference Specific Entropy
T	: Temperature
t	: Ton
$\mathbf{T_0}$	: Reference Temperature
U	: Internal Energy
$\mathbf{U_0}$	: Reference Internal Energy
V	: Volume
v	: Velocity
$\mathbf{V_0}$	: Initial Volume
$\mathbf{v_0}$	: Initial Velocity
$\mathbf{\dot{W}_{cv}}$	: Control Volume Work
$\mathbf{W_{aircooler}}$	: Air Cooler Work
$\mathbf{\dot{W}_{cv}^{rev}}$	: Reversible Control Volume Work
$\mathbf{w_i}$	: Aggregating Weight of i^{th} Neural Network Combination
$\mathbf{W_{NET}}$	: Net Work
$\mathbf{W_{pump}}$	: Pump Work
$\mathbf{X, x}$	: Neural Network Inputs Vector
$\mathbf{x_i}$	: Mole Fraction
z	: Elevation
$\mathbf{z_0}$	: Reference Elevation
$\boldsymbol{\beta_i}$	: Correction Factor
$\boldsymbol{\gamma_i}$	: Component Activity Coefficient
$\boldsymbol{\mu_{i0}}$	: Chemical Potential
$\boldsymbol{\mu_{i00}}$	: Equilibrium State of Chemical Potential
$\boldsymbol{\eta}$	: Energy Efficiency

Σ	**:** Sum
ψ	**:** Exergy Efficiency
0	**:** Reference Point
1,2,3	**:** States

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COMPUTER-AIDED EXERGY AND ENERGY ANALYSIS OF THE VACUUM DISTILLATION UNIT

SUMMARY

Recently, studies on energy efficiency have become very important due to greenhouse gas emissions, raw material costs and resource constraints. Energy efficiency encourages researchers to work on these issues in terms of both reducing costs and protecting the environment. In order to carry out energy efficiency studies, firstly, the sources that cause energy consumption should be analyzed, so that the necessary actions can be taken as a result of these analyzes. Among these actions, the options to be evaluated include studies such as recovery of process waste heat, prevention of unwanted leaks, evaluation of new technological possibilities, regular maintenance of equipment, as well as the implementation of designs and operations that will increase energy efficiency.

Refineries are complex energy-intensive industry that are both energy producers and consumers. For this reason, a wide-ranging energy management is required in refineries. Refineries consist of distillation columns that process crude oil to obtain different petroleum products. The refinery consists of units such as crude oil distillation, vacuum distillation, hydrocracker, catalytic cracking, hydrodesulfurizer, and isomerization. The unit where crude oil is first processed is the crude oil distillation unit. In the crude oil distillation unit, gas, LPG, light and heavy naphtha, kerosene, light and heavy diesel and finally atmospheric bottom products are obtained, respectively. These products can be sold directly or sent to other units to create new products in the refinery.

Atmospheric bottom products with a very high boiling point coming from the crude oil distillation unit are sent to the vacuum distillation unit for processing. It is ensured that the desired products are obtained without thermal decomposition by utilizing the boiling points drop of the products under vacuum pressure. In the vacuum distillation unit, atmospheric bottom products first pass through the preheat train and furnace to reach the desired charging temperature, and then are fed to the vacuum distillation column. From light to heavy, waste gas, light vacuum gas oil, heavy vacuum gas oil vacuum bottom product are obtained, respectively. The waste gas is cleaned in amine units and this cleaned gas used as fuel in the furnace. The other products obtained are intermediate products and sent to units such as catalytic hydrocrackers or hydrocrackers for processing.

Energy analysis is a traditional method for evaluating the performance of systems and is connected to the first law of thermodynamics known as conservation of energy. In addition, energy efficiency calculations and energy balances are used in the energy analysis method. However, energy balance cannot give any information about the degradation of energy resources. Therefore, energy analysis cannot measure energy losses and energy quality. In addition, energy efficiency calculations used to analyze the performance of the system can be misleading or confusing in some cases.

At this point, the exergy method copes with the limits of the first law of thermodynamics. Exergy is related to both the first law and the second law of thermodynamics. The second law of thermodynamics presents the concept of entropy, which expresses the disorder in the system. Accordingly, the total entropy of a system either increases or remains constant in any random process, but never decreases. Consequently, the second law of thermodynamics is concerned with the quality of the system corresponding to the conversion of energy into work. Exergy is defined as the maximum theoretical useful work that can be achieved as the system becomes completely thermodynamic equilibrium with its environment.

Exergy analysis is an important tool in determining the energy losses and measuring the quality of the process. Because there is always a degradation in energy quality for real processes. Therefore, exergy analysis results give meaningful results. At this point, exergy analysis studies provide information to designers, engineers and researchers about the performance of the system. At the same time, there are many useful studies about the exergy analysis in the literature to evaluate the performance of systems and to improve the performance of the system. Exergy has both system and reference environmental properties. If a system is in equilibrium with its environment, that system has no exergy and this is called a dead state. If the exergy of the system increases, exergy deviates from the environment. The total system exergy consists of a combination of potential, kinetic, physical and chemical exergy. Exergy can be transferred as mass, heat and work.

Exergy efficiency, one of the system performance indicators, measures the approach to ideal conditions. The higher the system has exergy efficiency, the higher there is energy quality of system. There are many equations related to exergy efficiency in the literature. It is usually expressed as the ratio of the sum of the output exergy to the sum of the input exergy. Exergy efficiency is always between zero and one. Another performance indicator is the expression of irreversibility or exergy waste, which indicates the deviation of the system from ideal conditions. This irreversibility expression can be calculated by the exergy balance or by using the relevant equations in the literature.

Some procedures should be followed in order to apply exergy analysis. At the beginning, the system to be examined is decided and if necessary, system elements can be evaluated separately. Required operational values such as temperature, pressure and flow are reached for exergy and energy calculations. Energy calculations are done using common mass and energy balances. For exergy analysis, a reference environment is selected and exergy calculations are done according to this reference. In addition, exergy balance is used to calculate the exergy consumption. Appropriate equations are also used for the exergy efficiency of the system. Finally, these calculated values are interpreted. Inefficiencies in the system are determined and actions are taken to improve system performance depending on the need.

There are many equipment in refineries that can be thermodynamically examined. These equipment can be heat exchangers, chillers, air coolers, furnaces, distillation columns, pumps and compressors. Simulation is an important tool for modeling refineries, and various software products were developed for this. One of them is ASPEN HYSYS, which is widely used. Thanks to the interactive platform provided by HYSYS, users set up and run their models effectively and quickly. In addition, ASPEN HYSYS provides comprehensive thermodynamic infrastructure to accurately calculate phase behavior, physical and transport properties for refining, oil or gas industries. HYSYS offers users many basic unit operations such as separators, reactors, rotary equipment, heat transfer and logical operations. It also provides a good environment for performing exergy and energy analysis calculations and performing various case studies in different operational conditions.

In this study, energy and exergy analysis of the vacuum distillation unit in TUPRAS Refinery was performed. The main purpose of the study is to discover the inefficiencies of all unit operations in the vacuum distillation unit with exergy analysis studies. In addition, these objectives include interpreting energy losses in operations with energy inefficiencies and identifying fields that may have potential for improvement. Another aim of the study is to see the effect of operational parameters on column exergy efficiency depending on the process control limits. Finally, the exergy efficiency prediction of vacuum distillation column was studied using machine-learning models. For this, parameters affecting the column were used as model inputs. The purpose of developing prediction models is to see and evaluate the results on the online platform without the need for the continuous ASPEN HYSYS working environment and intensive exergy calculations in the background. At the same time, it can be determined whether this operation is efficient or not for any operational condition by using the predictive models on the column.

In beginning, the study starts with a detailed literature search to understand the exergy concept and to reach the equations to be used in exergy calculations. Then, a vacuum distillation unit was simulated in ASPEN HYSYS in order to carry out energy and exergy studies. For the simulation, a base date which has all data was selected. Actual plant data were used for simulation. These data are laboratory values and operational values such as temperature, pressure and flow. In addition, the equipment technical reports were used in the simulation. Overall unit operations such as heat exchanger, heater, cooler, air cooler, pump, furnace and column was simulated in HYSYS. The comparison of the actual values with the HYSYS model results was made for each operational value. The model was updated continuously until actual values and model results converge. After the last accurate model simulation was obtained, exergy and energy analysis calculations were started. In exergy calculations, exergy transfer equations were taken into consideration. For mass or flow exergy calculations, calculations were done using the enthalpy, entropy, exergy values of the simulation streams and the equations in the literature. Also, the exergy efficiency calculations in the literature were done for each equipment. Equipment with low exergy efficiency was identified. Evaluations about where the performance degradation of these equipment may come from were done. In addition, the exergy and energy efficiency values of the equipment were compared. Moreover, the effect of the parameters on the column exergy efficiency was evaluated using the case study function of ASPEN HYSYS according to the process control limits. The most important parameters affecting the column exergy efficiency were determined.

Synthetic data was produced in ASPEN HYSYS by using the parameters that affect the column most. Prediction models were developed using this data set with machine learning methods. For this, BANN, which is one of the artificial neural network models, and Random Forest models, one of the ensemble learning methods, were developed in the R program. The "Ipred" and "randomForest" packages of the R program were used for BANN and the Random Forest model, respectively. The data for both models are divided into training, testing, and invisible validation data sets. The accuracy and success of the model was interpreted by looking at the fit between the last real values and the model predicted values.

VAKUM DİSTİLASYON ÜNİTESİNİN BİLGİSAYAR DESTEKLİ EKSERJİ VE ENERJİ ANALİZİ

ÖZET

Son zamanlarda sera gazı emisyonları, ham madde maliyetleri, kaynak sıkıntısı nedeniyle enerji verimliliği konulu çalışmalar oldukça önem arz etmektedir. Enerji verimliliği, hem maliyetleri azaltması hem de çevreyi koruması açısından araştırmacıları bu konularda çalışmalara teşvik etmektedir. Enerji verimliliği çalışmalarının gerçekleştirilmesi için öncelikle enerji tüketimine sebebiyet veren kaynakların analiz edilmesi gerekmektedir böylece bu analizler sonucunda gerekli aksiyonlar alınabilir. Bu aksiyonlar arasında değerlendirilmesi gereken seçenekler proses atık ısılarının geri kazanılması, istenmeyen kaçakların önlenmesi, yeni teknolojik olanakların değerlendirilmesi, ekipmanlarda düzenli bakımların yer alması aynı zamanda enerji verimliliğini yükseltecek tasarımların ve operasyonların uygulanması gibi çalışmalar yer almaktadır.

Petrol rafinerileri enerji yoğun karmaşık yapılar olup hem enerji üreticisi hem de tüketicisidir. Bu nedenle petrol rafinerilerinde geniş çaplı bir enerji yönetimi gereklidir. Rafineriler ham petrolü işleyerek farklı petrol ürünlerini elde eden distilasyon kolonlarından oluşmaktadır. Rafineri, ham petrol distilasyon, vakum distilasyon, hidrokraker, katalitik kraking, hidrodesülfürizer, izomerizasyon gibi ünitelerden oluşmaktadır. Ham petrolün ilk işlendiği ünite ham petrol distilasyon ünitesidir. Ham petrol distilasyon ünitesinde hafiften ağıra sırasıyla gaz, likit petrol gazı (LPG), hafif ve ağır nafta, kerosen, hafif ve ağır dizel ve son olarak atmosferik dip ürünleri elde edilir. Bu ürünler doğrudan satışı yapılmakla birlikte rafineride yeni ürünler oluşturmak için başka ünitelere gönderilebilir.

Ham petrol işleme ünitesinden elde edilen kaynama noktası çok yüksek olan atmosferik dip ürünler işlenmek üzere vakum distilasyon ünitesine gönderilir. Vakum basıncında ürünlerin kaynama noktalarının düşmesinden yararlanarak ısıl bozunmaya uğramadan istenilen ürünlerin elde edilmesi sağlanır. Atmosferik dip ürünler vakum ünitesinde öncelikle ön ısıtıcı ağlarından ve fırından geçerek istenilen şarj sıcaklığına getirilir ve vakum distilasyon kolonuna beslenir. Hafiften ağıra sırasıyla atık gaz, hafif vakum gaz yağı, ağır vakum gaz yağı vakum dip ürünü elde edilir. Atık gaz amin ünitelerinde temizlenerek tekrardan fırında yakıt olarak kullanılır. Elde edilen diğer ürünler ara ürün olup işlenmek üzere katalitik hidrokraker veya hidrokraker gibi ünitelere gönderilir.

Enerji analizi sistemlerin performansını değerlendirmede geleneksel bir yöntem olup enerjinin korunumu olarak bilinen termodinamiğin birinci kanunuyla ilişkilidir. Enerji analizi yönteminde enerji verimliliği hesaplamaları ve enerji denkliği işlemleri kullanılır. Bununla birlikte, kullanılan enerji dengesi, enerji kaynaklarının bozulması hakkında hiç bir bilgi veremez. Böylece enerji analizi, enerji kayıplarını ve enerji kalitesini ölçememektedir. Ayrıca sistemin performansını incelemek için kullanılan enerji verimliliği hesaplamaları bazı noktalarda yanlış yönlendirebilmekte veya kafa karışıklığı yaratabilmektedir.

Ekserji metodu bu noktada termodinamiğin birinci kanunu limitlerini aşmaktadır. Ekserji konsepti hem termodinamiğin birinci kanunu hem de ikinci kanunuyla ilişkilidir. Termodinamiğin ikinci kanunu sistemdeki düzensizliği ifade eden entropi kavramını sunar. Buna göre bir sistemin toplam entropisi herhangi bir rastgele süreçte ya artar ya da sabit kalır, asla azalmaz. Sonuç olarak termodinamiğin ikinci yasası enerjinin işe dönüşebildiği yani kalitesini ele almaktadır. Ekserji, sistemin çevresiyle tümüyle termodinamik denge haline gelirken elde edebilecek maksimum teorik yararlı iş olarak tanımlanır.

Ekserji analizi prosesteki enerji kayıplarını belirlemede ve prosesin kalitesini ölçmede önemli bir araçtır. Çünkü gerçek proseslerde her zaman enerji kalitesinde bir bozulma vardır. Bu nedenle ekserji analizi sonuçları anlamlı çıktılar vermektedir. Bu noktada ekserji analizi çalışmaları, tasarımcılara, mühendislere ve araştırmacılara sistemin performansı hakkında bilgi vermektedir. Aynı zamanda literatürde ekserji analizi kullanılarak sistemlerin performansını değerlendirmek ve sistemin performansını geliştirmek için birçok faydalı çalışma da bulunmaktadır.

Ekserji sadece termodinamik kavramın ötesinde hem sistem hem de referans çevre özelliklerine sahiptir. Bir sistem çevresiyle dengedeyse o sistemin ekserjisi yoktur ve bu durum ölü durum olarak adlandırılır. Eğer sistemin ekserjisi artarsa ekserji çevreden sapmaktadır. Toplam sistem ekserjisi potansiyel, kinetik, fiziksel ve kimyasal ekserjilerin birleşiminden oluşur. Ekserji kütlesel, ısı ve iş olarak aktarılabilir.

Sistem performans indikatörlerinden biri olan ekserji verimliliği ideal koşullara yaklaşımın ölçüsüdür. Ekserji verimliliği enerji verimliliğe göre sistemin performansını anlamada önemli bir araçtır. Sistem ne kadar yüksek ekserji verimine sahipse o kadar yüksek enerji kalitesine sahiptir. Literatürde ekserji verimliliği ile ilgili eşitlikler oldukça fazladır. Genelde, çıkış ekserjilerinin toplamının giriş ekserjilerinin toplamına oranı olarak ifade edilir. Ekserji verimliliği her zaman sıfır ile bir arasındadır. Diğer bir performans indikatörü ise sistemin ideal koşullardan sapmasını gösteren tersinmezlik ya da ekserji atığı ifadesidir. Bu tersinmezlik ifadesi ise ekserji dengesinden hesaplanarak ya da literatürde ilgili eşitlikler kullanılarak hesaplanabilir.

Enerji analizi çalışmalarında geleneksel olarak kullanılan enerji kavramı ile ekserji kavramı arasında farklılıklar vardır. Örneğin; enerji her zaman korunurken, ekserjide tersinmez veya gerçek prosesler için her zaman bir yıkım söz konusudur. Enerji sadece miktar ölçüsünü dikkate alırken, ekserji hem miktarı hem de kaliteyi ölçer. Enerji çevreden bağımsız olup ekserji çevre ile bağımlıdır.

Ekserji analizini uygulayabilmek için bazı prosedürler takip edilmelidir. Buna göre başlangıçta incelenmek istenen sisteme karar verilir, gerekirse sistem elemanları ayrı ayrı değerlendirilebilir. Ekserji ve enerji hesaplamaları için gerekli olan sıcaklık, basınç ve akış gibi operasyonel değerler elde edilir. Bilinen kütle ve enerji denklikleri kullanılarak enerji hesaplamaları yapılır. Ekserji analizi için ise bir referans ortamı seçilir ve bu referansa göre ekserji hesaplamaları yapılır. Ekserji tüketimlerini görebilmek için ekserji denkliği kullanılır. Sistemin ekserji verimliliği için de uygun eşitlikler kullanılır. En son hesaplanan bu değerler yorumlanır. Sistemdeki verimsizlikler belirlenir ve ihtiyaca bağlı olarak performansı iyileştirebilecek aksiyonlar alınır.

Petrol rafinerilerinde termodinamik olarak incelenebilecek birçok ekipman vardır. Bu ekipmanlar ısı değiştiriciler, soğutucular, havalı soğutucular, fırınlar, distilasyon kolonları, pompalar ve kompresörler olabilir. Petrol rafinerilerini modellemek için simülasyon önemli bir araçtır ve bunun için çeşitli yazılım ürünleri geliştirilmiştir.

Bunlardan biri yaygın olarak kullanılan ASPEN HYSYS'dir. Kullanıcılar, HYSYS'nin sağladığı interaktif platform sayesinde modellerini etkili ve hızlı bir şekilde kurar ve çalıştırır. Ek olarak, ASPEN HYSYS, rafinaj, petrol veya gaz endüstrileri için faz davranışını, fiziksel ve taşıma özelliklerini doğru bir şekilde hesaplamak için kapsamlı termodinamik altyapı sağlar. HYSYS kullanıcılara, ayırıcılar, reaktörler, döner ekipmanlar, ısı transferi ve mantıksal işlemler gibi birçok temel işlem seçenekleri sunmaktadır. Aynı zamanda ekserji ve enerji analizi hesaplamalarını yapmak ve farklı operasyonel koşullarda çeşitli durum çalışmaları gerçekleştirmek için de iyi bir ortam sunar.

Bu çalışmada TÜPRAŞ Rafinerisi'nde bulunan vakumlu damıtma ünitesinin enerji ve ekserji analizi yapılmıştır. Çalışmanın esas amacı enerji analizinin yanı sıra farklı bir kavram olan ekserji analizi çalışmaları ile vakum distilasyon ünitesinde yer alan tüm birimlerin verimsizliklerini keşfetmektir. Ayrıca, enerji verimsizlikleri görülen operasyonlarda enerji kayıplarının neden olabileceğini yorumlamak ve iyileştirme potansiyeli olabilecek alanları belirlemektir. Çalışmanın diğer amacı ise, vakum distilasyon kolonunun verimini arttırabilecek şekilde proses kontrol limitlerine bağlı olarak operasyonel parametrelerin ekserji verimliliği üzerinde etkisini görmektir. Son olarak, makine öğrenmesi modelleri kullanılarak vakum distilasyon kolonunun ekserji verimliliği tahmini üzerinde çalışılmıştır. Bunun için kolonu etkileyen parametreler model girdisi olarak kullanılmıştır. Tahmin modelleri geliştirmenin amacı ise, arka planda sürekli ASPEN HYSYS çalışma ortamına ve yoğun ekserji hesaplamalarına gerek kalmadan canlı platformda sonuçları görebilmek ve değerlendirmektir. Aynı zamanda kolon üzerinde geliştirilen tahmin modelleri ile herhangi bir operasyonel koşul için bu operasyonun verimli olup olmadığını belirlenebilir.

Çalışma ilk olarak ekserji konseptini anlamak adına ve ekserji hesaplamalarında kullanılacak eşitliklere ulaşmak için detaylı bir literatür araştırmasıyla başlamaktadır. Daha sonra enerji ve ekserji çalışmalarını gerçekleştirmek için ASPEN HYSYS'te vakum distilasyon ünitesi simülasyonu yapılmıştır. Simülasyon için tüm verilerin ulaşılabildiği bir baz tarihi alınmıştır. Simülasyon için gerçek ünite verileri kullanılmıştır. Bu veriler laboratuvar değerleri ve sıcaklık, basınç ve akış gibi operasyonel değerlerdir. Ayrıca ekipmanlara ait ekipman teknik raporunda yazan bilgiler de ünite simülasyonunda kullanılmıştır. Ünitede yer alan ısı değiştirici, ısıtıcı, soğutucu, havalı soğutucu, pompa, fırın ve kolon gibi tüm birim operasyonların simülasyonu HYSYS'te yapılmıştır. Gerçek değerler ile HYSYS model sonuçlarının karşılaştırılması sıcaklık, basınç ve akış gibi her operasyon değer için yapılmıştır. Gerçek değerler ile model sonuçları yakınsayana kadar model sürekli güncellenmiştir. En son doğru model simülasyonu elde edildikten sonra ekserji ve enerji analizi hesaplamalarına başlanmıştır. Ekserji hesaplamalarında ekserji aktarımı eşitliklerine dikkat edilmiştir. Kütlesel ya da akış ekserji hesaplamaları için simülasyon akımlarına ait entalpi, entropi, ekserji değerleri ve literatürde yer alan eşitlikler kullanılarak hesaplamalar yapılmıştır. Aynı zamanda her ekipman için literatürde bulunan ekserji verimliliği hesabı yapılmıştır. Ekserji verimliliği düşük olan ekipmanlar belirlenmiştir. Bu ekipmanların performans düşüşlerinin nereden kaynaklanabileceğine ait değerlendirmeler yapılmıştır. Bununla birlikte ekipmanlara ait ekserji ve enerji verimlilik değerlerinin karşılaştırılması yapılmıştır. Ayrıca, proses kontrol limitlerine göre kolonu kontrol eden parametrelerin ekserji verimliliği üzerine etkisi ASPEN HYSYS'in durum çalışması fonksiyonu kullanılarak değerlendirilmiştir. Kolonun ekserji verimini etkileyen en önemli parametreler belirlenmiştir.

Ekserji verimliliğini etkileyen parametreler değerlendirildikten sonra bu parametreler kullanılarak ASPEN HYSYS'te sentetik veri üretilmiştir. Makine öğrenmesi yöntemleri ile bu veri seti kullanılarak tahmin modelleri geliştirilmiştir. Bunun için yapay sinir ağı modellerinden biri olan Torbalama ve topluluk öğrenmesi metotlarından biri olan Rassal Orman modelleri R programında geliştirilmiştir. R programının "Ipred" ve "randomForest" paketleri, sırasıyla Torbalama ve Rassal Orman modeli için kullanılmıştır. Her iki modelin verileri eğitim, test ve görünmeyen doğrulama veri setlerine ayrılmıştır. Bu bölünme eğitim seti için %50, test seti için %30 ve görünmeyen doğrulama veri seti için %20 olacak şekildedir. En son gerçek değerler ile model tahmini değerler arasındaki uyuma bakılarak modelin doğruluğu ve başarısı yorumlanmıştır.

1. INTRODUCTION

Nowadays industries face with economic and environmental difficulties in terms of global warming, source scarcity as well as enhanced raw material and energy cost that press on companies to applying sustainability strategies. Energy efficiency and reducing energy usage are important issues for the sustainability of companies [1]. Energy efficiency has many positive factors for industries thanks to developing productivity, decreasing environmental damage and reducing the operating cost [2].

The industries cause 36% global energy consumption and 35% global greenhouse gas emission because they are a big energy consumer. The oil and gas industry is both major manufacturer and consumer of energy. According to IEA report, oil refineries are responsible for 9% of energy consumption in Figure 1.1. The refinery operations that are resource extraction, processing, transformation and transportation extending to delivery to end users require a large energy consumption [2, 3]. Therefore, evaluating petroleum industry in energy analysis studies is critical.

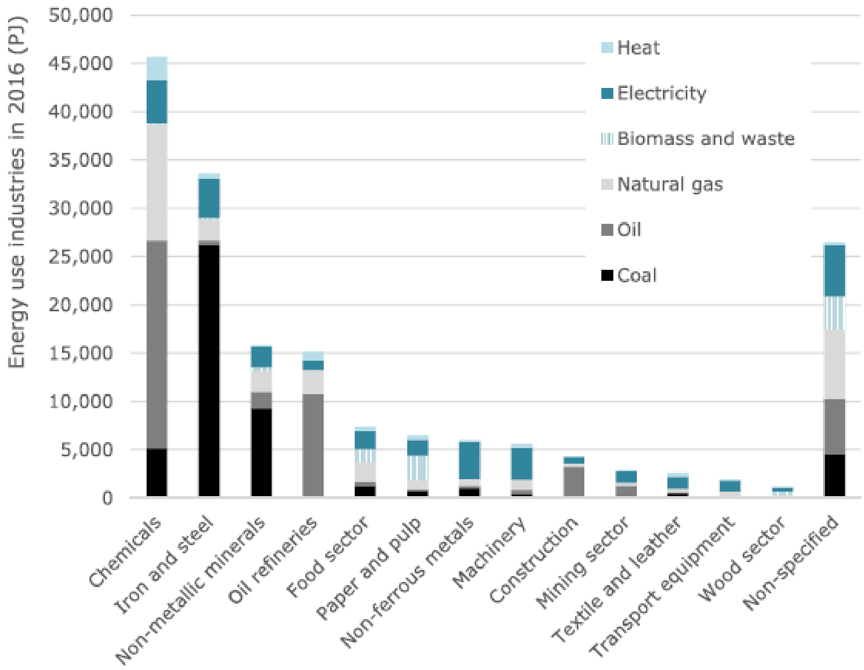


Figure 1.1: Global energy usage in industries [3].

When energy is used as measuring tool to comprehend and develop energy efficiency, misdirection and confusion might happen in some cases. The quantity exergy provides more understandable and useful information in terms of evaluating the waste in energy systems compared to the information provided by energy [4].

Exergy term is related with both the First Law of Thermodynamics (FLT) and the Second Law of Thermodynamics (SLT). The FLT is known as the energy conservation law that means even though energy can change state; it might be neither created nor exterminated. Exergy analysis technique, which depends on the SLT, cope with the FLT limitations. The Second Law of Thermodynamics identifies the principal quantity entropy, which represents the unavailability of randomized energy form to convert work directly. Also, it states that all physical and chemical spontaneous processes increase the entropy [5].

The exergy analysis can be used in different fields that can be shown in Figure 1.2.

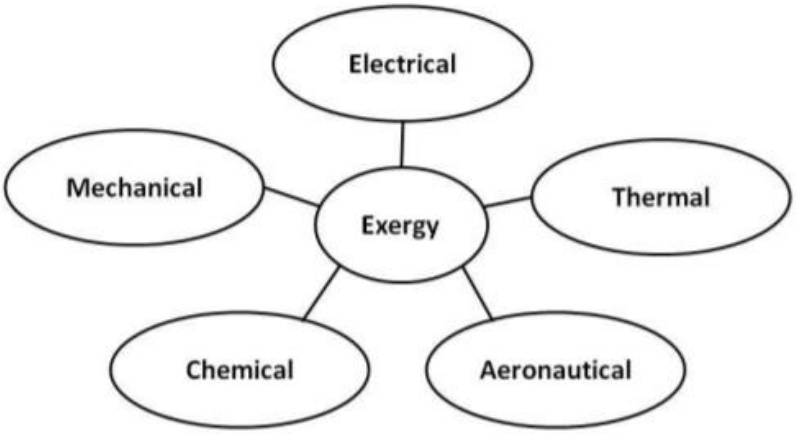


Figure 1.2: Fields sharing exergy [6].

In addition to this, there are many kinds of exergy process applications on energy systems like industrial, utility, transportation as well as residential-commercial. The usage of exergy analysis can mainly be applied to industrial energy processes. Due to the plenty of different energy usage, determination of overall efficiency is complicated for the industrial sector that can be grouped as petrochemical, chemical process (chemical production, water desalinization, distillation, etc.), metallurgical process like lead smelting and the systems of heating and cooling. Since exergy method is a powerful tool in terms of analyzing, evaluating, designing, developing and optimizing process and system, it is used in various industries. Process steam, mechanical driving force, direct and space heating are some of the energy consumptions in the industrial sector. In the utility sector, not only conventional energy resources including fossil and nuclear, but also renewable resources including geothermal, biomass, wind, solar and water are used for processes of electricity production. In addition, residential, public, commercial and agribusiness activities are involved the sector of residential-commercial that uses different energy carriers [7, 8].

There are many different field of applications about usage of exergy methods in the literature. For instance, Dong et al. presented that the exergy analysis method provides theoretical information about improving engine performance, reducing fuel usage and optimizing engine combustion for aircraft systems, turbojet and scramjet engines [9]. Fellaou et al. implemented the exergy analysis of desalination facility. They found largest degradation in the module of membrane, the high-pressure pump and delivery pump that were 64.28%, 40.84% as well as 38.48% respectively. [10]. In another research, energy and exergy calculations were conducted to the process of biomass gasification of pinewood, horse manure and sawdust for hydrogen production using the gasifying agents. In comparison with results, higher hydrogen exergy efficiency is obtained with steam gasification for pinewood. When the exergy efficiency of product gas reached the top value (88.26%), the exergy efficiency of hydrogen was obtained as 44% [11]. Bai et al. compared the energy and exergy analysis between the cycle systems of developed supercritical CO_2 and existed supercritical CO_2 for coal power station. Whole exergy efficience of the developed supercritical CO_2 cycle was found 2.32% more than the existed supercritical CO_2 cycle [12]. In other research, an exergy analysis of marine gas turbine system was conducted for per system element and entire system. It was concluded that among the all heat exchangers, while combustion gases heat exchangers had the maximum exergy efficiencies, cooler had the minimum exergy efficiency. It was also discovered that the turbines have higher exergy efficiency than compressors. The exergy efficiency of the entire process was 64.12% [13]. Bühler et al. carried out energy and exergy methods to investigate a production facility of milk powder. The spray dryer and the gas burner had the maximum exergy destruction and low exergy efficiencies were appeared in the heaters [14].

Considering the petroleum sector that are responsible for high energy consumption, the crude oil distillation units have many constituents which are the furnace, the distillation towers and heat exchanger networks with respect to applying energy and exergy methods thermodynamically. Therefore, many researchers focused on different components for the exergy analysis studies in the refinery.

One of these studies is the exergy analysis in a crude oil fractionating column. Al-Muslim et al. carried out exergy analysis of petroleum refining units with one and two stage, which comprised of furnace and fractionating column for identifying exergy degradations and efficiencies. The effect of reference condition on exergy performances of petroleum refining units with one and two-stage was examined in another study. This study pointed out that the increment of exergy losses occurred while the reference temperature increased and thus the exergy efficiency decreased [15, 16]. Tarighaleslami et al. examined the atmospheric refining column in Tabriz Refinery for a case study to see the feasibility of different retrofit choices in the way of thermodynamic exergy loss studies. The best retrofit option was found reduction in exergy loss of 17.16%, resulting in 3.6% reduction in fuel demand [17]. Gu et al. employed exergy analysis on three crude oil vacuum distillation columns to assist designers in process choice. This study provided an output to see appropriate furnace exit temperature and process depending on the expected purposes of the unit [18]. In another research, multi-stage impact on crude distillation with using energy and exergy thermodynamically was investigated. It resulted with diminution in the exergy and energy of heat demand of crude distillation unit occurred when the number of stage increased [19]. Dincer and Rosen researched operation parameters effects including temperature and pressure of the crude oil refining column on system efficiencies using exergy method. As a result, the changes in temperature and pressure profile did not give rise to important change on the efficiencies of energy and exergy especially for vacuum distillation unit [20].

Pre-distillation unit containing various heat exchanger networks and furnaces are also used in exergy analysis studies. For instance, Vilarinho et al. executed both energy and exergy studies of the pre-distillation unit in Portuguese Refinery. Overall efficiency results were obtained as 13.4% energy efficiency and 2.3% exergy efficiency in pre-distillation unit. Also, both energy and exergy losses of furnace were found 15.6% and 56.3% in the unit [21]. Izyan and Shuhaimi applied exergy analysis for performance assessment of the crude preheating network and furnace inside the petroleum distillation unit. The presented options for decreasing exergy loss in this study were cleaning schedule of preheat network and heat loss reduction from furnace [22].

Computer aided studies such as process simulation, machine learning models are important methods for both energy and exergy analysis in terms of evaluating process analysis, design and optimization. Osuolale and Jie Zhang studied with thermodynamic tools using ASPEN simulation program and artificial neural network model in order to help both engineers and designers in terms of designing and operating energy efficient crude oil distillation units [23]. Osuolale and Jie Zhang also applied exergy analysis on distillation column for binary systems by means of using artificial neural network in another research. 32.4% increment of exergy efficiency was occurred with changing the operating conditions without causing additional investment costs [24].

In this research, exergy analysis of vacuum distillation unit (VDU) that composed of heat exchanger network, furnace and distillation column in TUPRAS Refinery was investigated. Computer aided simulation of VDU was done in order to examine exergy analysis in ASPEN HYSYS v10 with using equipment, laboratory and operational data. Both energy and exergy calculations were accomplished for all unit operations such as pumps, furnace, heat exchangers, air coolers, and vacuum distillation column. The exergy efficiency in the column has been studied specially. The impact of various operation parameters on column exergy efficiency analyzed by using "Case Study" of ASPEN HYSYS. In addition, machine learning (ML) models for column exergy efficiency were improved using process operation data from simulation. Due to intensive exergy calculation, the success of ML model predictions were examined by using two models to satisfy online working environment. In addition to presentation of exergy analysis studies in the vacuum distillation column, examination the operational variables affecting the column exergy efficiency is among the aims of this study. Furthermore, exergy analysis is supported neural network models to enhance model accuracy and reliability.

2. DESCRIPTION AND SIMULATION OF PROCESS

2.1 Description of Process

The first step of refinery is crude oil distillation that separates crude oil into various petroleum products known as fractions according to the boiling temperature difference. Distillation plant comprises of two petroleum distillation towers, which are the atmospheric and vacuum tower. While the light hydrocarbons are distinguished in atmospheric tower, the heavy hydrocarbons are distinguished in vacuum tower. Although, vacuum tower has the same operating basis with atmospheric tower, it has fewer stages and side cuts [20].

In this study, vacuum distillation unit in TUPRAS Refinery was evaluated as a case study. The VDU consists of four mainly unit parts such as feed preheat section, vacuum distillation unit furnace, vacuum distillation unit column with pump-around (PA) circuits and amine units. The basic representation of the VDU is in Figure 2.1. The aim of the VDU process is to separate the atmospheric residue by three main streams consisting of light vacuum gasoil (LVGO), mixture of medium and heavy vacuum gas oil (MHVGO) as well as vacuum residue (VR). Sour water, waste gas, slops oil and Heavy Slop Oil (HSO) are also obtained in this process.

2.1.1 Feed preheat section with heat exchanger network

The heat exchanger network (HEN) performs two targets that are chilling of product streams and preheating of the atmospheric crude oil. Shell and tube type heat exchangers take part in the HEN.

The HEN comprises five unit heat exchangers. Initially, atmospheric residue, which is cold feed from tank, is sent to VDU for preheating against product stream in the first heat exchanger. Also, hot atmospheric residue from the available crude distillation units is sent to stream of first heat exchanger exit. These two atmospheric residues mix before feeding into the second heat exchanger. Then, this mixed atmospheric residue is preheated against PA stream in the second heat exchanger. Exit stream of second heat exchanger splits two branches. A branch is routed to third heat exchanger to preheat against PA stream and other branch is routed to fourth heat exchanger to preheat against return stream. Two branches that are exit of third and fourth heat exchangers are mixed with each other. Finally, mixed stream is routed to fifth exchanger to preheat against VR.

2.1.2 Vacuum distillation unit furnace

Atmospheric crude oil residues from the exit of fifth heat exchanger is heated in the VDU furnace using fuel gas. The atmospheric crude oil residues start vaporizing with combustion. Then, the partially vaporized atmospheric residue mixture is transferred into the vacuum distillation column.

2.1.3 Vacuum distillation unit

The vacuum distillation unit is operated with vacuum pressure to provide separating heavy hydrocarbons and enable to less temperature for distillation of crude oil. Series of ejectors is placed to create vacuum pressure. The scheme representing the vacuum distillation column is shown in the Figure 2.1.

In this model, a fifteen-stage vacuum distillation column is assumed for simulation. Vapor of atmospheric residue coming from furnace is charged at fourteenth stage number. Also, stripping stream is introduced at fifteenth stage. The vacuum distillation column has four side cuts involving light components to heavy components respectively are light vacuum gas oil (LVGO) at third stage, medium vacuum gas oil (MVGO) at ninth stage, heavy vacuum gas oil (HVGO) at eleventh stage, heavy slop oil (HSO) at thirteenth stage. The overhead product at first stage is sent to amine system for gas cleaning. The vacuum residue is taken from the fifteenth bottom stage. The VDU has four PA circuits, which are cold LVGO PA, LVGO PA, MVGO PA and HVGO PA.

The PA circuits remove the heat from the VDU. Liquid is drawn from a specific tray, is cooled in the heat exchangers and is returned at a lower temperature to the tray above the tray, which is drawn liquid, by the PA circuits. They are described with the drawn and the return stage, the return temperature as well as the mass rate of flow.

2.1.4 Amine units

The VDU overhead product that is called off gas stream can contain high concentration of H_2S. It is treated in amine units before sent to the VDU furnace for burning. The amine units have three sections such as amine absorber, amine regenerator and amine filtering. Amine absorber removes the H_2S of vacuum off gas. Amine regenerator regenerate the amine by removing the H_2S. Amine filters remove corrosive products and other contaminants from the amine.

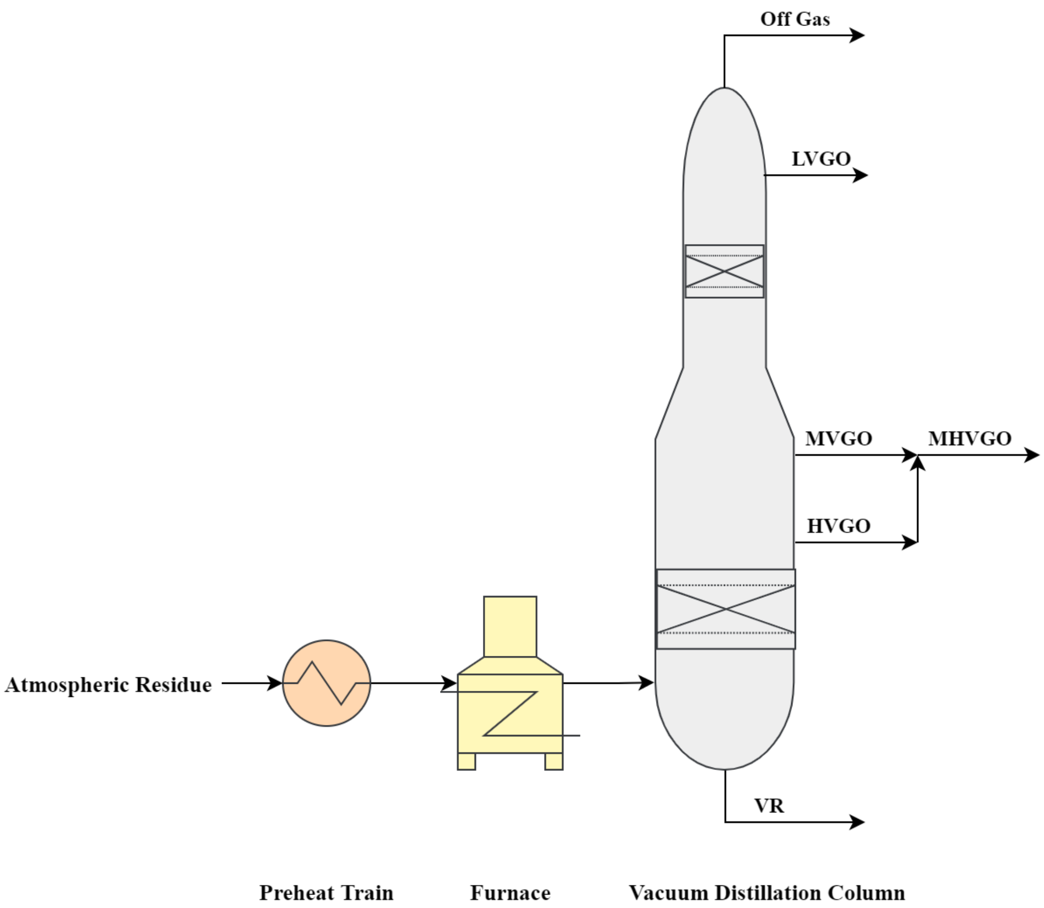


Figure 2.1: Scheme of the vacuum distillation unit.

2.2 Process Simulation

Various software products that simulate and optimize the refining process were developed for the petroleum industries. One of them is ASPEN HYSYS, which is commonly used. Users set up and work their models effectually and quickly by provided interactive platform of HYSYS. In addition, ASPEN HYSYS enables extensive thermodynamic substructure to calculate phase behavior, physical and transport properties for the refining, oil and gas industries accurately. There are many unit operations such as separators, reactors, rotating equipment, heat transfer and logical operations in HYSYS. Not only the steady state modeling but also dynamic modeling are done in this environment [25].

ASPEN HYSYS consists of property and simulation environments that present customized user interfaces to carry out different tasks. The properties environment shows entire configuration tasks of basic physical characteristics connected with a simulation. Work streams associated with obtaining, regression and estimation of the property data as well as calculated properties with customized methods and models are involved in the property environment. The simulation environment is used to build and utilize process models. It has many functions to make and modify a flowsheet of process as well as examine this process [26].

To develop ASPEN HYSYS flowsheet for petroleum refining process, some procedures that indicated below have to be followed:

1. Component list is created in the properties environment.

2. Fluid package is selected in the properties environment.

3. Assay characterization of atmospheric residue from the laboratory data is made in the properties environment.

4. Process flow diagram (PFD) of VDU is improved in the environment of simulation.

    a. Unit operations are specified with the input and output material streams, energy streams as well as required operational and design conditions.

    b. The feed flowrates are specified with flowrates, compositions and operating conditions such as temperature, pressure and vapor fraction.

5. Running the simulation of VDU to produce data for exergy analysis occurs in the simulation environment.

In summary, ASPEN HYSYS workflow diagram for petroleum distillation process is viewed in Figure 2.2.

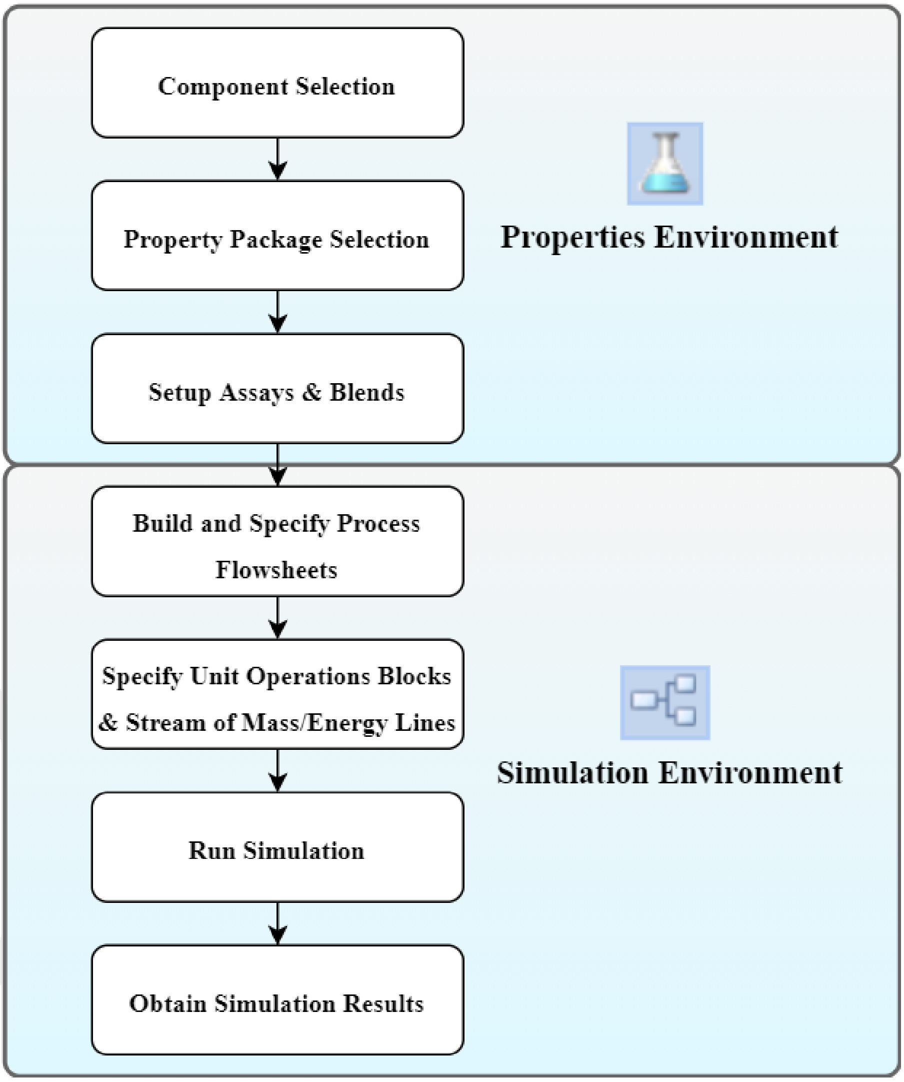


Figure 2.2: ASPEN HYSYS workflow diagram for petroleum distillation process.

2.2.1 Defining the components and the property models

When ASPEN HYSYS V10 opens, new button is chosen. The initial step of the simulation is the creating of component list. Figure 2.3 shows the component list tabs. If the add button is clicked in the component list tabs, the database list which has pure and hypothetical components will appear in Figure 2.4.

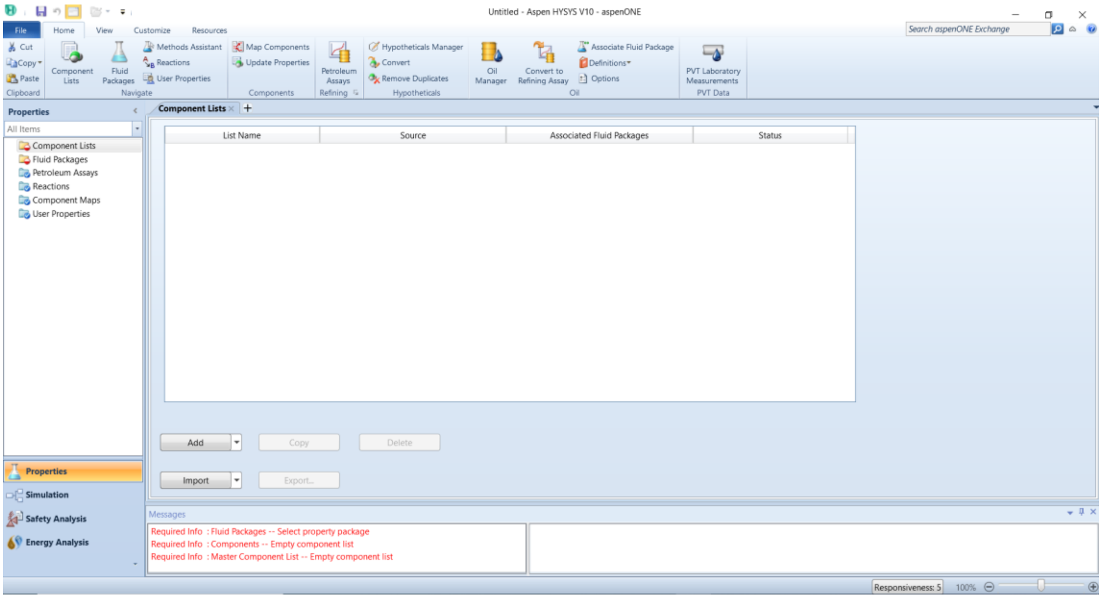


Figure 2.3: ASPEN HYSYS component list tabs.

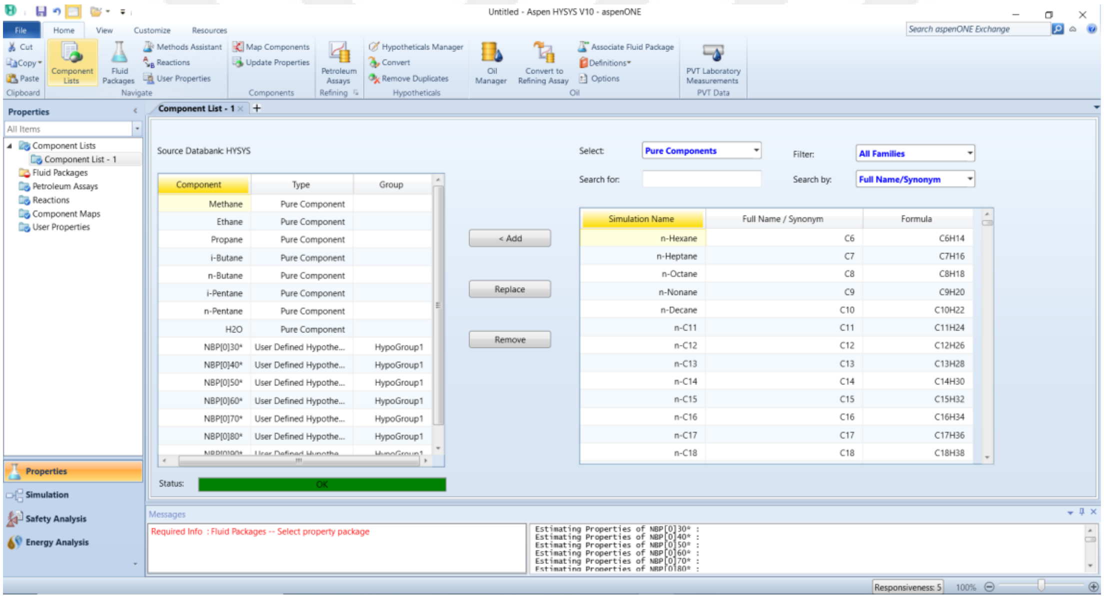


Figure 2.4: Source databank in the component list tabs of ASPEN HYSYS.

A large amount of unknown hydrocarbons chemicals and compounds form the content of crude oil. Because of the inadequate information about the crude oil content, it is frequently qualified in relation to the boiling point of hypothetic constituents [27].

2.2.2 Defining the fluid package

After describing the component list, fluid packages are created with clicking add button from fluid packages tabs. Appropriate thermodynamic model is selected between many options and it is ensured that thermodynamic model is related with Component List - 1. The “decision or selection tree” shown in Figure 2.5 can be used for the choice of the most appropriate thermodynamic package. Some physical properties of compounds included in the process to decide the thermodynamic model. These properties are polarity, electrolyte, pressure and real or pseudo constituents. The Peng Robinson (PR), which is one of the equation of state (EOS), is mostly preferred among the property packages for petroleum, oil and gas process because of containing nonpolar or little polar and real components. In addition, the PR Fluid Package is improved in terms of comprising wide range of pressure and temperature, great database of binary interaction as well as being particular behaviour for key ingredients [28].

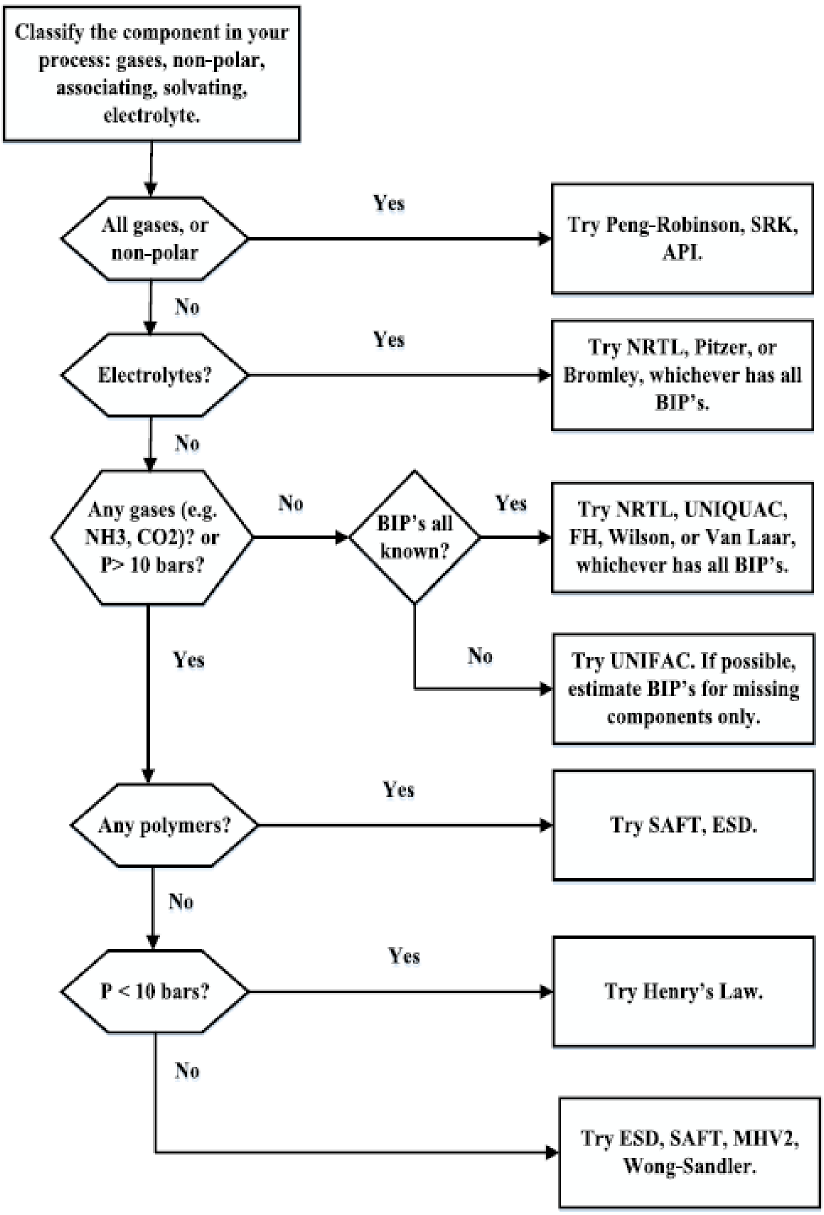


Figure 2.5: Selection of proper thermodynamic model considering decision tree [28].

Also, appropriate fluid package selection can be made with the help of methods assistant in the property environment of ASPEN HYSYS shown in Figure 2.6. According to component or process type in the method assistant, this selection is decided.

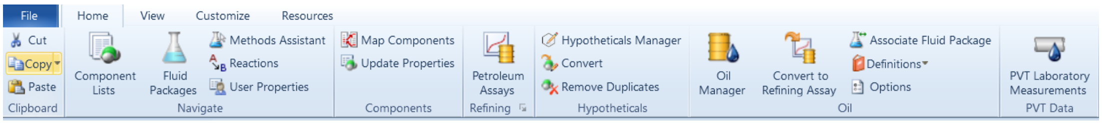


Figure 2.6: Methods assistant for selecting appropriate thermodynamic model.

Peng-Robinson, Antoine and ASME Steam model were used as thermodynamic fluid packages. Figure 2.7 shows Peng-Robinson model selection from fluid packages tabs. Peng-Robinson model is appropriate for oil and gas processing, Antoine model is recommended for petroleum assay at vacuum conditions and ASME steam model is used for defining the H_2O component in ASPEN HYSYS.

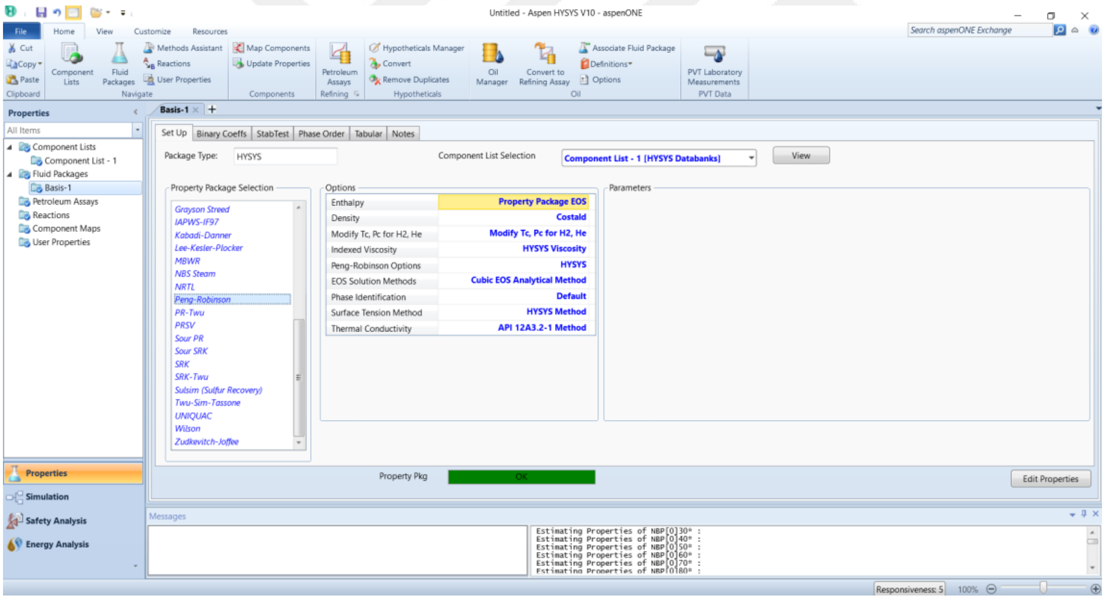


Figure 2.7: Fluid packages tabs of ASPEN HYSYS.

2.2.3 Assay characterization of atmospheric residue

Petroleum has all type of hydrocarbons mixture such as aliphatic, aromatic etc. with salts, water, sulfur and nitrogen including compositions and metal complexes. Hence, alternative methods are available for characterizing petroleum like density and distillation curves instead of using composition directly. Crude oil is characterized by utilizing American Society for Testing and Materials (ASTM) and True Boiling Point (TBP) methods. TBP curves estimate about the properties and composition of the crude oil and is plotted between the boiling point of all component of the mix and cumulative volume percent of distilled. Due to its features of time consuming and costly, another quicker method was proposed such as ASTM. One of ASTM methods is ASTM D86 that is used for nearly entire petroleum fractions except for heavy distillations [29].

In this study, a summary day that holds exact laboratory data was selected to simulate the unit. Distillation values for this summary day were entered into the simulation. Atmospheric residue petroleum assay was created by back blending of the VDU products which consist of LVGO, MVGO, HVGO and VR (Figure 2.8).

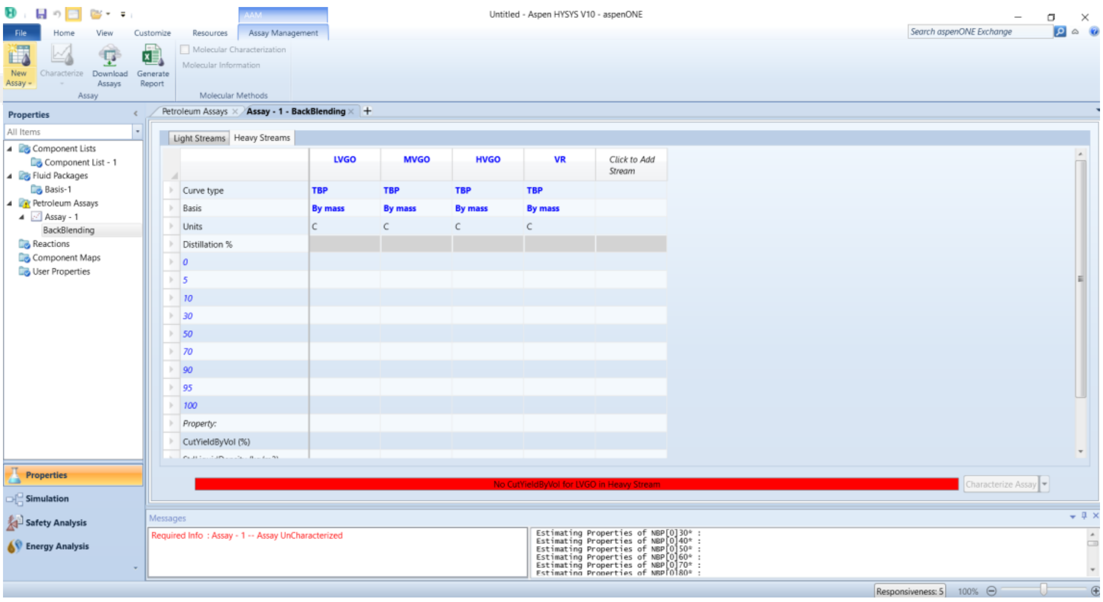


Figure 2.8: Back blending of atmospheric residue from assay tabs.

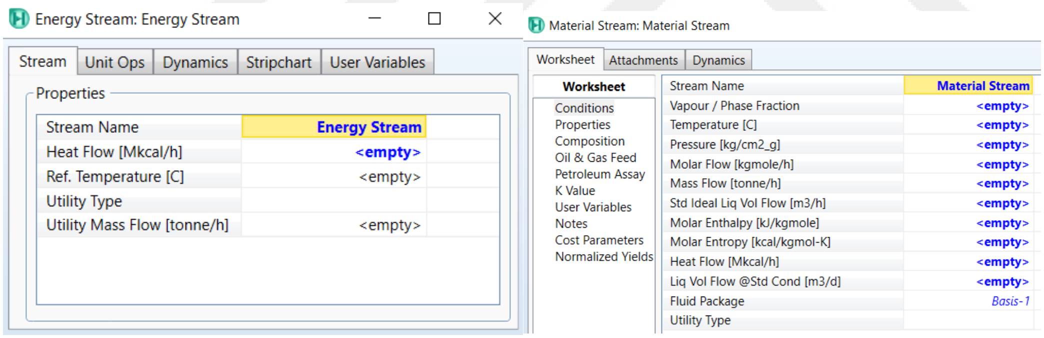
Average tagged unit operation values of selected summary day such as flow, temperature and pressure values were used in order to create process flow diagram of VDU. Moreover, equipment design values of each equipment belonging to the unit were entered into the simulation with using equipment data sheet. After the improvement of PFD, the simulation was run. The comparison was made between the result of simulation and operation conditions for summary day to check the accuracy of the simulation. Finally, the simulation was used for exergy analysis.

2.2.4 Building and specifying process flowsheet

Creating process flowsheet takes place in the simulation environment of ASPEN HYSYS. Streams are necessary between all unit operations. For VDU, the model process simulation consists of heat exchanger network for preheat section, VDU furnace and vacuum distillation column.

2.2.4.1 Material and energy streams

Material streams travelling input and output of simulation boundaries and proceeding among unit operations can be simulated in ASPEN HYSYS. The properties and composition of material streams must be specified in order to be solved by HYSYS. While describing material streams, degrees of freedom is used to operate flash calculation by HYSYS. Therefore, composition and two process specifications required for flash calculation. These two specifications can be temperature, pressure, vapor fraction, enthalpy, and entropy, but between two process specifications, one of them must be either temperature or pressure. Also, one of the flow options is entered to define a material stream completely. In addition to this, energy streams travelling input and output of simulation boundaries and proceeding among unit operations can be simulated in ASPEN HYSYS. Figure 2.9 displays both the view of material and energy stream property [30].



(a) (b)

Figure 2.9: A screen of (a) Energy (b) Material stream in ASPEN HYSYS.

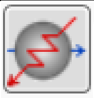
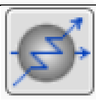
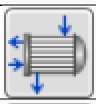
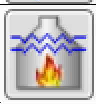
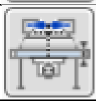
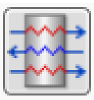
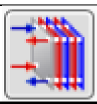
2.2.4.2 Unit operation blocks

There are many unit operations used to build flowsheets. These unit operations split up categories that contain many individual operations. For example, unit operation blocks can be classified as heat transfer equipment, piping equipment, rotating equipment, separators, reactors, logicals and user-defined blocks. While modeling operations, a degrees of freedom (DOF) approach is used by HYSYS [30].

Heat transfer operations

ASPEN HYSYS has many unit operations that are indicated in Table 2.1 for heat transfer modelling. Heater and Cooler are one side of an exchanger that can be used for heating or cooling, condensing or evaporating and changing pressure. Duty and pressure drop specifications are necessary in order to solve fully for the Heater and Cooler in ASPEN HYSYS. Heat transfers between two flows are modelled in the heat exchangers calculating two-sided material and energy balance. Heat exchanger model can be selected depending on user's analysis in Figure 2.10. Two specifications are essential to be solved by heat exchanger but detailed heat exchangers such as rating and rigorous models also need exchanger geometry information besides two specifications. One of these specifications is shell and tube side pressure drops. Other specification can be one of these specifications: product stream temperature, minimum temperature approach, overall UA, LMTD or temperature change. Air Cooler uses air for heating or cooling a process flow by some specified conditions that are pressure drop and overall UA. Also, air or process exit stream can be specified instead of overall UA [30].

Table 2.1: Heat transfer operations.

	Name	Description
	Heater	Simple heater specified via outlet stream temperature, dT, or heater duty
	Cooler	Simple cooler specified via outlet stream temperature, dT, or heater duty
	Heat Exchanger	Transfers heat between two streams
	Fired Heater	Direct fired heater furnace
	Air Cooler	Cools feed to meet an exit stream condition using an ideal air mixture
	LNG Heat Exchanger	Model heat transfer for heat exchangers with multiple stream specified via UA, waste heat or temperature approaches
	Plate Exchanger	Models heat transfer between two fluids using metal plates

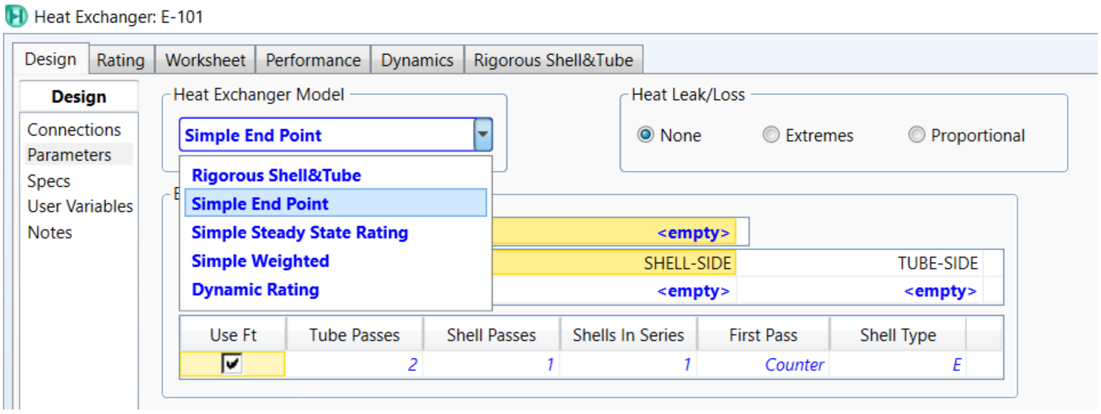
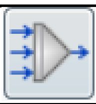
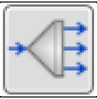
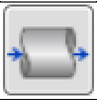
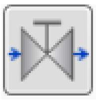
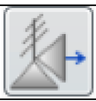


Figure 2.10: Heat exchanger model selection.

Piping operations

Piping operations of ASPEN HYSYS can be classified as individual operations giving in Table 2.2. The Mixer performs a complete balance of heat and material. If the all inlet streams properties such as pressure, temperature and composition are known, the outlet stream properties are calculated automatically in the Mixer. There are two specification for the Mixer related to pressure in Figure 2.11. If one of the connected stream pressure is entered, when "Equalize All" option from parameters tab of Mixer is selected, the same pressure is obtained in the entire connected streams. If all the stream pressures are known and they are different, "Set Outlet to Lowest Inlet" from parameters tab of Mixer should be chosen so the lowest inlet pressure for the outlet stream pressure is assigned. In addition, the Tee is specified by the desired flow ratio as Figure 2.12. Before the Control Valve operation solves, three specifications are necessary. They can be listed as input temperature and pressure, output temperature and pressure or pressure drop but two of them must be temperature and pressure specification. A wide sort of piping is simulated by using the Pipe Segment with estimation of heat transfer. It also presents pressure drop correlations [30].

Table 2.2: Piping operations.

	Name	Description
	Mixer	Blends multi inlet flows to generate one outlet flow
	Tee	Split one inlet feed flow into multi outlet flows for the same conditions and compositions
	Pipe Segment	Simulates single or multiphase piping
	Control Valve	Controls flow, decreases pressure, and performs a flash calculation; Supports sizing and rating
	Relief Valve	Models spring loaded relief valves; prevents pressure buildup and supports all phases

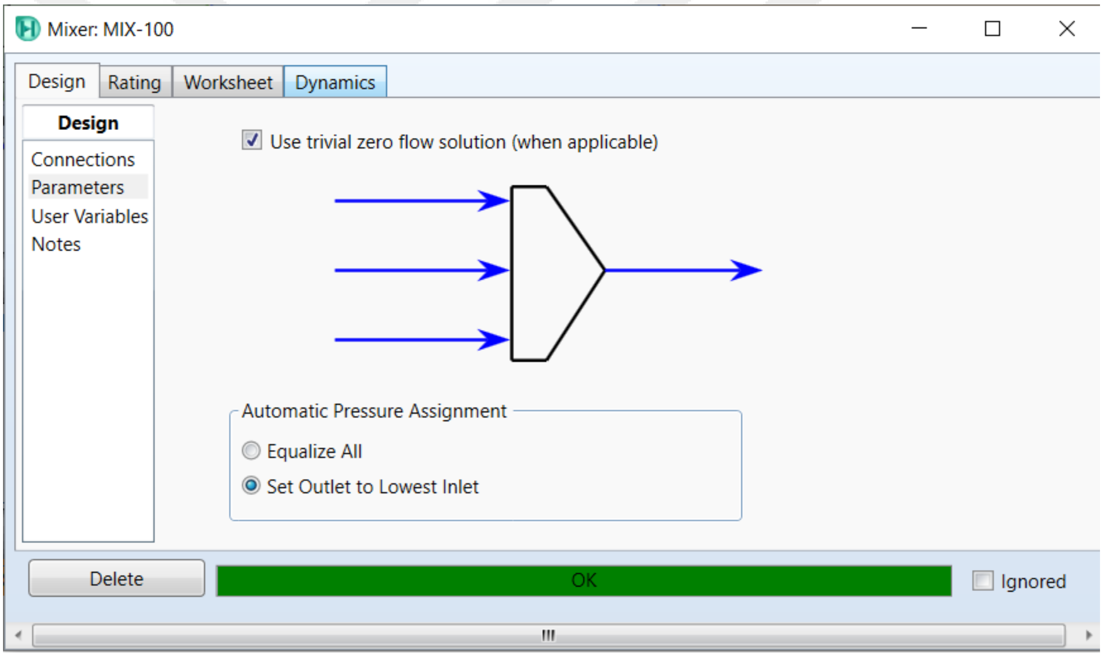


Figure 2.11: Pressure specification of the Mixer.

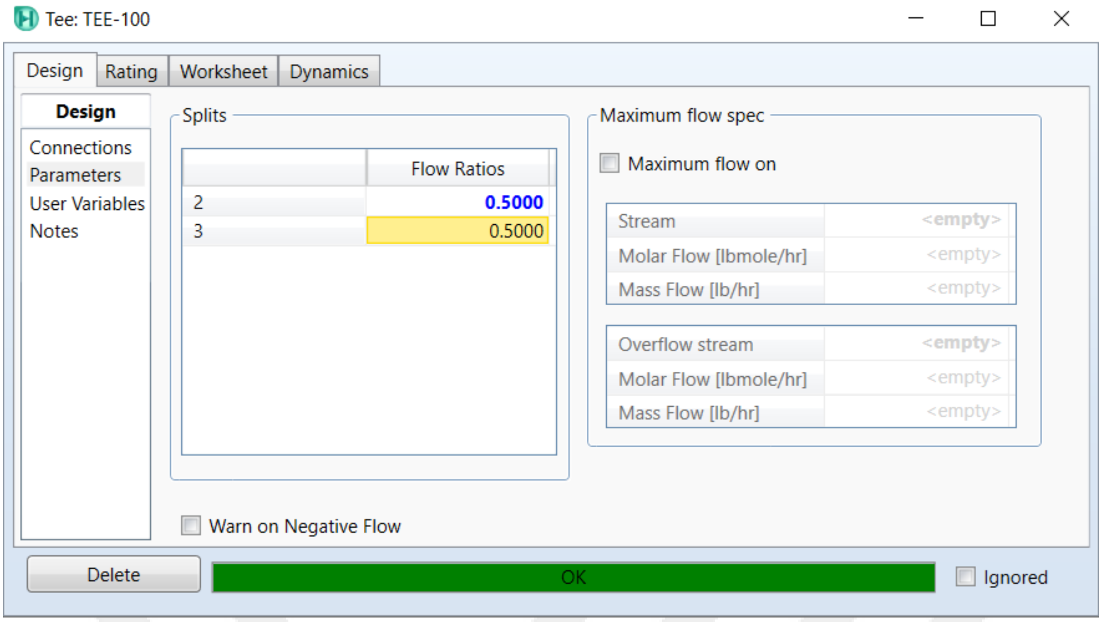
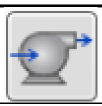
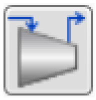
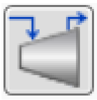


Figure 2.12: Flow ratios specification of the Tee.

Rotating operations

Different type of rotating operations are defined in Table 2.3. The Pump and Centrifugal Compressor calculate either an unknown temperature, pressure or efficiency based on the information specified by user. If the inlet stream is fully described, just two of the variables should be specified for both the Pump and Centrifugal Compressor: outlet pressure or pressure drop, energy and efficiency. Unlike the Centrifugal Compressor, the Expander creates outlet stream with high velocity and low pressure. The gas internal energy is converted into kinetic energy and eventually converted into shaft work by an expansion process. To conclude, while compression process needs energy, expansion process releases energy [30].

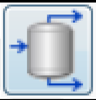
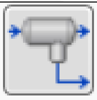
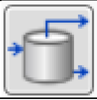
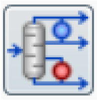
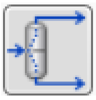
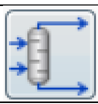
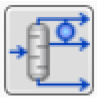
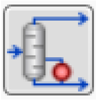
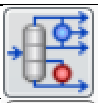
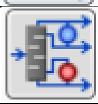
Table 2.3: Rotating operations.

	Name	Description
	Pump	Increases the pressure of a liquid stream; Calculates pressure, temperature or efficiency
	Compressor	Model centrifugal, reciprocating and screw compressors. Increases pressure of inlet gas; Calculates stream condition or efficiency
	Expander	Centrifugal expander decreases pressure of inlet gas; Calculates stream condition or efficiency

Separation and column operations

ASPEN HYSYS offers many types of separation and column operation in Table 2.4. The views of property for the Separator, 3 Phase Separator, and Tank are similar. The essential differences in the three separator operations are the stream connections that are described in Table 2.4. The first step in setting up the Column is to decide which type wanted depending on the equipment of Column like reboiler or condenser. Column build environment of HYSYS is specified with column configurations including side strippers and pump arounds sections [30].

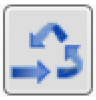
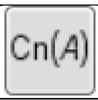
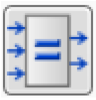
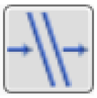
Table 2.4: Separation operations.

	Name	Description
	Separator	Separates vessel components into vapor and liquid states; Supports multi feed streams
	3 Phase Separator	Separates vessel components into vapor and two liquid states; Supports multi feed streams
	Tank	Models fluid surge vessels; Separates vessel components into vapor and two liquid states
	Distillation Column	Distillation column sub-flowsheet with a condenser and reboiler; Supports side-draws, side-strippers and pump-arounds
	Blank Column	Empty column sub-flowsheet that can be configured with side operations, condensers, reboilers, etc.
	Component Splitter	Separates feed components into multiple product streams based on TBP, split fractions, etc.
	Absorber	Absorber column sub-flowsheet; Supports side-draws, side-strippers and pump-arounds
	Refluxed Absorber	Absorber column sub-flowsheet with a refluxed condenser; Supports side-draws, side-strippers and pump-arounds
	Reboiled Absorber	Absorber column sub-flowsheet with a reboiler; Supports side-draws, side-strippers and pump-arounds
	3 Phase Distillation	Divides vessel contents into vapor and two liquid phases; Supports multiple feeds
	Shortcut Column	Carries out short cut calculation for basic refluxed towers

Logical operations

Logical operations constitute relationships logically between the components that compose the process without physically performing calculations of heat and material balance. Table 2.5 shows some logical operations. In case a flowsheet does not have a direct solution, a definite combination of specifications may be necessary. The method of trial-and-error must be used for solving of this kind of problems. These trial-and-error iterations are conducted by the Adjust operation automatically. The Spreadsheet operation performs user-defined calculations that are linked with flowsheet variables. If flowsheet variables change, the cells of Spreadsheet are updated. A Recycle operation is required, when downstream material streams mix with upstream material streams [30].

Table 2.5: Logical operations.

	Name	Description
	Adjust	Changes the value of one input variable to meet a targeted specification on one calculated variable
	Spreadsheet	Used to perform custom calculations, manipulate flowsheet variables, organize data, etc.
	Recycle	Assists in a solver convergence loop by transferring stream conditions to the next iteration
	Set	Be utilized for defining a process variable value with respect to another process variable
	Balance	Balances a set of stream inlets and outlets based on moles, mass, heat, mole and heat, or mass and heat
	Stream Cutter	Performs a fluid package transition, or switch. Allows transfer of information from one stream to another on a different fluid package.

3. STUDY OF THE ENERGY AND EXERGY ANALYSIS

The analysis of energy is a thermodynamic method based on FLT that is linked to the conservation of energy principle. However, the method of exergy is connected with the both FLT and SLT. While conservation of energy rule known as the FLT, nonconservation of entropy rule known as the SLT. The method of exergy can be used to specify and quantify exergy destruction of process owing to the exergy losses and irreversibility. Therefore, it is alternating and informative tool in terms of evaluating and comparing systems and processes. In comparison to energy analysis, exergy analysis presents more meaningful efficiencies and identifies the thermodynamic losses more clearly. The detailed comparison for energy and exergy is given in Table 3.1. Also, the same general equations can be written for both of them in any control volume [1, 4, 31].

Table 3.1: Comparing of energy and exergy [5].

Energy	Exergy
Result of the FLT, conserved for entire processes	Result of the SLT, conserved as two-sided processes (reversible), not conserved for actual processes
Only quantity measure	Quantity and quality measure
Seems many forms such as kinetic and potential energy, heat and work, plus is measured with these forms	Seems many forms such as kinetic and potential energy, heat and work, plus as is measured based upon work or ability of work producing
Is not produced and destroyed	Is not produced and destroyed for reversible process, but is destroyed for irreversible process
Takes values other than zero when it is in equilibration with the environment	Equals to zero while in balance with the environment that is named as dead state
Relates only an energy or a material flow features and independent of environmental features	Relates both an energy or a material flow features and the environment features

3.1 The Exergy Concept

The compounds of specified reference surroundings and system do a maximal shaft work that is defined as the exergy of a system. Also, exergy can be described as some words such as available energy, useable energy and availability. Exergy has meaning beyond a thermodynamic property; it has the characteristics of both the reference surrounding and a system. When a system provides a condition of equilibrium with its environment, there is not exergy for system. If exergy diverge from the environment, the exergy of system rises [5].

To understand the different forms of exergy, some state definitions should be explained [32]:

Process state: The beginning state of the system under a work is indicated by the process state (T, P).

Environmental state: The balance of mechanics and heat between the surroundings and the system is defined as the state of restricted equilibrium. System and ambient conditions such as pressures and temperatures are equal in the restricted equilibrium. Environmental state is described as a condition that satisfies the restricted equilibrium with the surroundings (T_0, P_0).

Dead State: Chemical potentials of the matters are required within the unrestricted equilibrium, including temperature and pressure of the system and surroundings to equal for providing thermodynamic balance totally between the surroundings and the system. Under these circumstances, the system exergy amount is equal to zero since the system cannot be exposed to any state changes during interaction with surroundings. This system state names as the dead state.

The exergy concept presents a global standard of energy quality in a specific environment. Exergy forming from the energy component may be converted to work for the reversible process but the energy quality reduces every time for real processes. Therefore, the exergy output is lower than its exergy input. This exergy equilibrium informs about the amount of exergy lost to the process. In other words, these exergy losses also named as irreversibility rate that are equal to degradation measure of the energy quality [19, 33].

While analyzing the thermodynamic of the system, three valid equations are used generally. These equations are the conservation of both energy and mass as well as the nonconservation of entropy equation. Some assumptions for deriving these equations are made as follows [15, 16, 20, 34]:

1. There is a system in steady flow states.

2. Reference state conditions are defined as P_0 = 101 kPa and T_0 = 298.15 K.

3. Changes in the potential and kinetic energies are ignored.

These simplifications are applied for three equations. They are the mass, energy, as well as exergy balance equations shown in equations 3.1, 3.2 and 3.3 respectively:

$$\sum_i \dot{m}_i = \sum_e \dot{m}_e \tag{3.1}$$

$$\sum_i \dot{E}_i + \dot{Q}_{cv} = \sum_e \dot{E}_e + \dot{W}_{cv} \tag{3.2}$$

$$\sum_i \dot{Ex}_i + \sum_j (1 - \frac{T_0}{T_j})\dot{Q}_{cv} = \sum_e \dot{Ex}_e + \dot{W}_{cv} + \dot{I}_{cv} \tag{3.3}$$

For the streams in equations 3.1, 3.2 and 3.3, $\dot{m}$ indicates the rate of mass flow, $\dot{E}$ indicates the energy rate and $\dot{E}x$ indicates the exergy rate. $\dot{Q}_{cv}$ is the rate of heat into a control volume, $\dot{W}_{cv}$ is the work done on the part of a control volume, $\dot{I}_{cv}$ is irreversible exergy loss of a control volume as well as inlet and exit of the stream are stated by the subscripts i and e in equations 3.1, 3.2 and 3.3. Also, the exergy losses from the control volume can be expressed as equation 3.4:

$$\dot{I}_{cv} = \dot{W}_{cv}^{rev} - \dot{W}_{cv} \tag{3.4}$$

3.2 The Exergy of Closed Systems

A closed system of mass exergy is stated as nonflow exergy. Equation 3.5 shows the nonflow exergy that is consisted of physical, chemical, kinetic, and potential exergy configurations [35].

$$Ex_{nonflow} = Ex_{ph} + Ex_o + Ex_{kin} + Ex_{pot} \tag{3.5}$$

Where

$$Ex_{pot} = g(z - z_0) \tag{3.6}$$

$$Ex_{kin} = \frac{1}{2}(v^2 - v_0^2) \tag{3.7}$$

$$Ex_o = \sum_i (\mu_{i0} - \mu_{i00})N_i \tag{3.8}$$

$$Ex_{nonflow,ph} = (U - U_0) + P_0(V - V_0) - T_0(S - S_0) \tag{3.9}$$

Terms of system in equations 3.6-3.9 correspond to velocity v, gravity acceleration g, elevation z, chemical potential μ_i and moles number N_i, pressure P, temperature T, internal energy U, volume V, entropy S with equilibrium state of T_0, P_0 and μ_{i00}. Also, μ_{i0} is equal to the value of μ where the environmental state. The subscript i denotes the species.

The maximum acquired work from the system is known as physical nonflow exergy while it comes to the ambient state. For instance, it is a condition of thermal and mechanical balance with the surroundings [35].

A maximum acquired work from the system is known as chemical nonflow exergy while it comes from an ambient condition to a dead condition. To illustrate, it is a condition of overall balance with the environment [35]. Equation 3.10 calculates a mixture chemical exergy [36-38].

$$ex_{mix}^{ch} = \sum x_i\, ex_i^{ch} + RT_0 \sum x_i\, ln(\gamma_i x_i) \tag{3.10}$$

Where x_i, ex_i^{ch}, γ_i and R indicate the mole fraction, chemical exergy, the i^{th} component activity coefficient as well as molar gas constant, respectively.

The first term of the equation 3.10 that is shown ex_i^{ch} is used for specified components. This term can not be used directly for the mixture of petroleum components. Standard chemical exergy for the light petroleum components in reference temperature and pressure can take part in literature. Therefore, they can be substitute for chemical exergy ex_i^{ch}. Since the mixture of heavy petroleum fraction can not be known exactly, it is separated into pseudo-components that need to be calculated depending on the lower heating value with equation 3.11 [38-40].

$$ex_i^{ch}(pseudocomponents) = LHV_i \beta_i \tag{3.11}$$

β_i is described as the correction factor of the i-th component chemical exergy as well as equation 3.12 shows the β that is related to mass fractions of C, H_2, O_2, S, and N_2 [36, 37, 39, 40].

$$\beta = 1.0401 + 0.1728\frac{z_{H_2}}{z_C} + 0.0432\frac{z_{O_2}}{z_C} + 0.2169\frac{z_S}{z_C}\left(1 - 2.0628\frac{z_{H_2}}{z_C}\right) + 0.0428\frac{z_{N_2}}{z_C} \tag{3.12}$$

Where z_C, z_{H_2}, z_{O_2}, z_S, and z_{N_2} correspond to mass fractions of C, H_2, O_2, S, and N_2 respectively. LHV is also calculated by equation 3.13 [41].

$$LHV\ [\frac{MJ}{kg}] = 55.5 - 14.4.SG \tag{3.13}$$

Specific gravity is expressed as SG in equation 3.13.

3.3 Exergy of Flows

Exergy might be transferred to system through mass, heat and work, as well as exergy might be transmitted from a system.

3.3.1 Exergy of material flow

Summation of a non-flow exergy and a stream work exergy is equal to the exergy of a material flow as following equation 3.14 [35]:

$$Ex_{flow} = Ex_{nonflow} + (P - P_0)V \tag{3.14}$$

If equation 3.5 is placed in equation 3.14 without chemical, kinetic, and potential exergy components, equation 3.15 is obtained. Also, if equation 3.15 is rearranged, equation 3.16 is reached. Equation 3.16 corresponds to the equation 3.17 that is known as the physical exergy flow of stream. It is stated as the enthalpy and entropy differences from the conditions of stream to reference.

$$Ex_{flow} = (U - U_0) + P_0(V - V_0) - T_0(S - S_0) + (P - P_0)V \tag{3.15}$$

$$Ex_{flow,ph} = (U + PV) - (U_0 + P_0V_0) - T_0(S - S_0) \quad (3.16)$$

$$Ex_{flow,ph} = (H - H_0) - T_0(S - S_0) \quad (3.17)$$

Where H and H_0 represent the enthalpy for stream and reference conditions, as well as S and S_0 represent the entropy for stream and reference conditions, respectively in equations 3.15, 3.16 and 3.17.

3.3.2 Heat exergy

Exergy is transferred by heat when a control volume, which is initially dead state, is heated or cooled in interactions with another system. If the exergy flow correlates with heat transfer Q, Ex_Q in equation 3.18 expresses this exergy flow [35].

$$Ex_Q = \int_i^f \left(1 - \frac{T_0}{T}\right) \partial Q \quad (3.18)$$

The interval of integral of equation 3.18 shows the situation from initial (i) to the final situation (f), as well as ∂Q and T_0 are equal to incremental heat transfer and environmental temperature, respectively. When temperature is constant, then equation 3.18 becomes as equation 3.19.

$$Ex_Q = \left(1 - \frac{T_0}{T}\right) Q \quad (3.19)$$

3.3.3 Work exergy

Exergy is transferred by work when a system does the work because of the volume change in time between t_1 and t_2. This is expressed by $(W_{NET})_{1,2}$ as equation 3.20 [35].

$$(W_{NET})_{1,2} = W_{1,2} - P_0(V_2 - V_1) \quad (3.20)$$

Where $W_{1,2}$ states the system work because of volume changing (V_2 – V_1) and translocation work is stated by $P_0(V_2 - V_1)$. Work exergy stream equates to work related to specified energy form. Therefore, shaft work consisting of both mechanical and electrical work is equal to exergy.

3.4 Energy and Exergy Efficiency

Engineers measure the performances of tools and processes with using efficiencies. These numerous expressions are depended on energy that is related to FLT. Moreover, SLT based efficiencies are useful in terms of considering limitations that is stemming from performance measures. When energy input is equal to energy output, there is a maximum efficiency in the process. Nevertheless, energy based efficiency can misdirect because of its inability to criterion of approach to ideality. The SLT takes into account the criterion of approach to ideality. Maximum efficiency is stated as a reversible process that imply achieving an ideal for this law. Furthermore, considering the energy efficiencies, they can be bigger than a hundred percent like coefficient of performance. However, exergy efficiency is always between zero and a hundred percent [5, 42].

3.4.1 Energy efficiency

The expression of energy output divided by energy input indicates overall energy efficiency that can also be expressed in relation to energy loss in equation 3.21.

$$\eta = \frac{Energy\ output\ in\ product}{Energy\ input} = \frac{\sum_i H_{out}}{\sum_i H_{in}} = 1 - \frac{Energy\ loss}{Energy\ input} \qquad (3.21)$$

3.4.2 Exergy efficiency

The process exergetic performance is measured by exergy efficiency, which is a well-known index. According to different requirements and aims, several descriptions of exergy efficiency are available in the literature. Various authors suggested exergy efficiency equations for different processes. When defining the exergy efficiency, some terms can be used like “exergy output”, “exergy input”, “useful product” and “exergy expenditures” [18, 43]. Lior and Zhang [44] proposed two main class of exergy efficiency definitions as the total and the task exergy efficiencies:

(1) The result obtained with dividing the total output flow exergy by the input flow exergy is called as the total, overall, universal or input-output exergy efficiency.

(2) The output obtained with dividing exergy statements coming from the generated products inside the system to exergy statements coming from expended resources is

called as the task, rational, utilitarian functional or consumed-produced exergy efficiency [44, 45].

3.4.2.1 Inlet-outlet exergy efficiency

The inlet-outlet efficiency exergy shown with equation 3.22 is described as dividing the total exergy output by the sum of exergy input or in another saying; it equals the ratio of net amount of generated exergy to net amount of provided exergy. Moreover, the exergy efficiency might be determined regarding the exergy losses [18, 45, 46].

$$\psi = \frac{\sum Exergy\ out}{\sum Exergy\ in} = \frac{Exergy\ output\ in\ product}{Exergy\ input} = 1 - \frac{\sum Exergy\ loss}{\sum Exergy\ input} \tag{3.22}$$

3.4.2.2 Consumed-produced exergy efficiency

There are five different exergy efficiency definition in consumed-produced class [47]. However, many exergy efficiency balances as well as exergy-based indicators can be presented at literature [43, 45, 48].

Grassmann [49] suggested a common expression for exergy yield that is the ratio of desirable exergy production to reducing of utilized exergy as equation 3.23.

$$\psi_1 = \frac{Useful\ Exergy\ Output}{Useful\ Exergy\ Input} \tag{3.23}$$

Kotas [50] used equation 3.24, which is called rational efficiency to specify the exergy performance, which equals the ratio of desired outputs to required inputs.

$$\psi_2 = \frac{Desired\ Output}{Necessary\ Input} \tag{3.24}$$

Szargut et al. [51] expressed that exergy performance equaled to the ratio of useful products exergy to feeding exergy in equation 3.25.

$$\psi_3 = \frac{Exergy\ of\ Useful\ Products}{Feeding\ Exergy} \tag{3.25}$$

Another definition of exergy efficiency is suggested by Brodyansky and Sorin as indicated in equation 3.26, which is the ratio of subtracting the total exergy input from the transit exergy to subtracting the whole exergy output from the transit exergy [52].

The exergy part supplied to the system as well as passing through the system, which does not undergo any physical and chemical change, is defined as transit exergy.

$$\psi_4 = \frac{Exergy\ Out - Transit\ Exergy}{Exergy\ In - Transit\ Exergy} \tag{3.26}$$

Tsatsaronis et al. [53] introduced the exergetic efficiency that is the ratio of the desired exergetic outlet to driving exergetic inlet. In other words, it is the ratio of products exergy to fuel exergy as indicated equation 3.27.

$$\psi_5 = \frac{Exergy\ of\ Products}{Exergy\ of\ Fuel} \tag{3.27}$$

3.5 Exergy Losses

There is always a degradation of energy quality in real processes. In comparison with the exergy output of process, the exergy input of process is always greater. The gap between them is described as exergy loss in equation 3.28 and 3.29. Destruction of exergy is known as exergy consumption that is resulted from irreversibility in a closed system. Figure 3.1 also shows the destruction of exergy considering to exergy balance. The more entropy is created, the more exergy is consumed. Equation 3.30 expresses this direct proportion between consumption of exergy and entropy creation. Exergy is destroyed as a positive value for any irreversible process, but it is zero for two-sided process known as reversible. It is pointed out equation 3.30. [19, 35].

$$Exergy\ loss = Exergy\ input - Exergy\ output \tag{3.28}$$

$$I = \sum Ex_{in} - \sum Ex_{out} \tag{3.29}$$

$$I = T_0 S_{gen} \geq 0 \tag{3.30}$$

Where I and S_{gen} indicates the exergy consumption and the entropy generation in a closed system respectively.

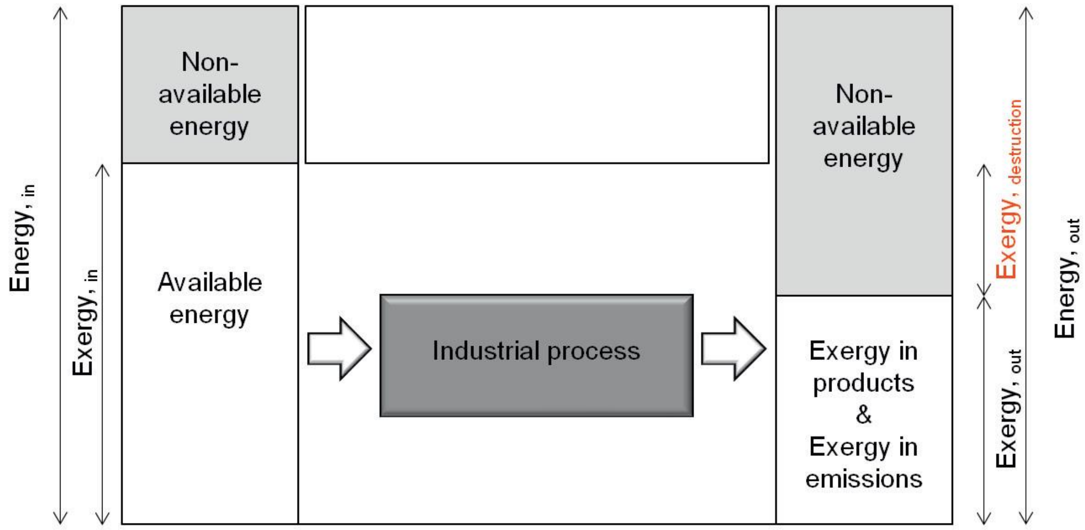


Figure 3.1: Balance of energy and exergy [1].

Exergy losses evaluate the deviations from ideality quantitatively. The location, sort, and reason of a waste or inefficiency are also determined by exergy losses. This information is important in terms of providing the way to increase exergy efficiency. Exergy losses connects two types of situation such as external and internal losses. These are related with residuals of exergy effluents and inner irreversibilities arising from exergy consumptions in a process or system [42]. These external losses can be contain as heat transfer with the environment (coolers utilizing air, water), unused energy component of material flows (exhaust and purge gases) and diffusion of heat losses from pipelines and operation equipment. However, spontaneous processes like combustion, limited driving and dissipative forces give rise to irreversibilities known as internal losses [47].

On the purpose of clarifying definitions of exergy efficiency, mathematical expressions are proposed for unit operations like compression, heat exchange, expansion, separation, mixing, as well as cyclic processes like heat engines and pumps [47]. Table 3.2 shows the exergy lost and exergy efficiency equations for some process equipment.

Table 3.2: The equations of exergy lost and exergy efficiency representing some unit operations [20, 32, 54, 55].

Unit Operation	Exergy Lost	Exergy Efficiency
Pump	$Ex_{in} - Ex_{out} + W_{pump}$	$\frac{Ex_{in} - Ex_{out}}{W_{pump}}$
Two-streams heat exchanger	$(Ex_{hot,in} - Ex_{hot,out}) - (Ex_{cold,out} - Ex_{cold,in})$	$\frac{Ex_{cold,out} - Ex_{cold,in}}{Ex_{hot,in} - Ex_{hot,out}}$
Heater	$Ex_{in} - Ex_{out} + Q$	$\frac{Ex_{out} - Ex_{in}}{Q}$
Air cooler	$\sum Ex_{in} - \sum Ex_{out} + W_{aircooler}$	$\frac{W_{aircooler}}{\sum Ex_{in} - W_{aircooler}}$
Column	$\sum Ex_{in} - \sum Ex_{out} + Ex^{Q}_{utility}$	$\frac{\sum Ex_{in} + Ex^{Q}_{utility} - I_{column}}{\sum Ex_{in}}$

4. MACHINE LEARNING MODELS

Machine learning (ML) permits computer programs to carry out complicated works such as planning, prediction, recognition and diagnosis with learned from historic data. ML model performance depends on data and algorithms. The size of large and high quality data can generally increase ML model accuracy. Applying appropriate algorithms is also important for solving various problems consisting of different types of datasets. The types of ML are divided into four categories such as supervised learning (SL), unsupervised learning (UL), semi supervised learning (SSL) and reinforcement learning (RL) as shown in Figure 4.1. The task of ML can be regression, classification, data reduction, clustering and anomaly detection as given in Figure 4.2 [56].

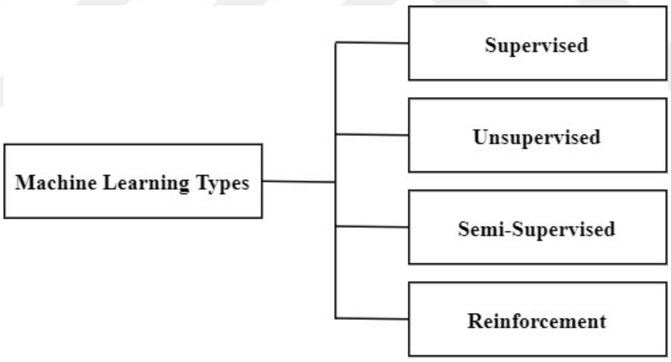


Figure 4.1: The types of ML [56].

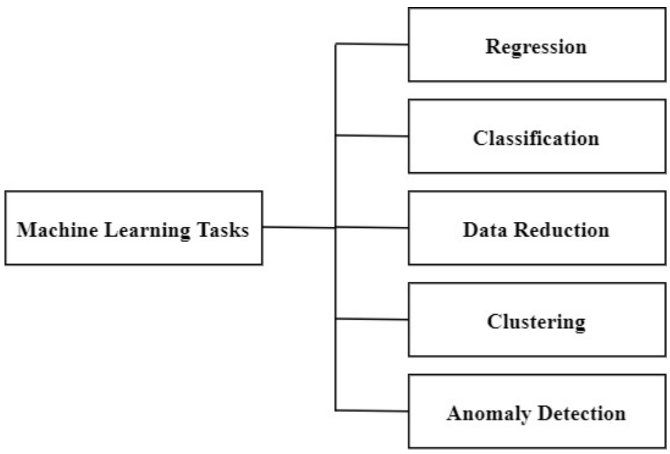


Figure 4.2: The tasks of ML [56].

For SL, the computer program trains the algorithm between input and output using a fully set of labeled data. Some of the SL algorithms are Regression, Decision Trees, Logistic Regression, Random Forest, K Nearest Neighbors (KNN) etc. In contrast to SL, UL does not use labeled data to train algorithm. Clustering algorithms such as K-mean and Hierarchical are the examples of UL. SSL that is the mixture of SL and UL develops a model using both data of labeled and unlabeled. RL enables agents to examine the environment using feedback mechanism from its self-actions. Online games such as backgammon and Atari are the examples of RL. Figure 4.3 shows the detailed classification of ML algorithms [56, 57].

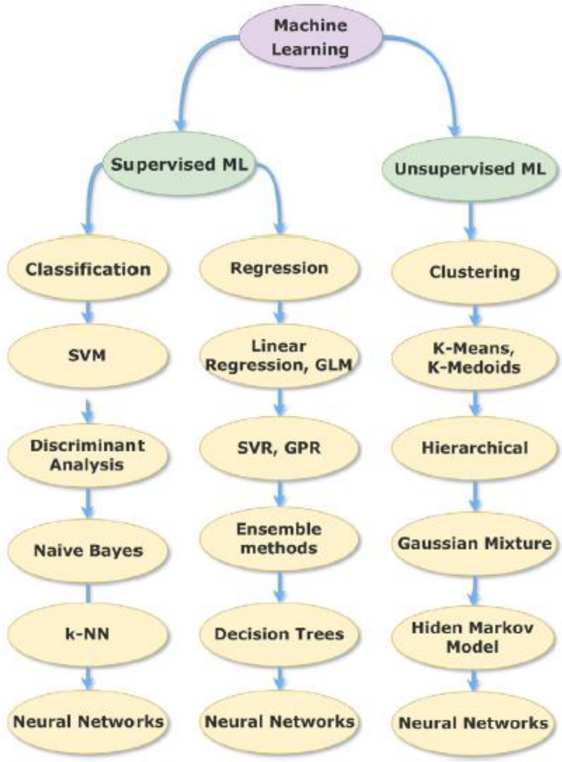


Figure 4.3: The classification ML algorithms [57].

In this study, two different machine-learning algorithms were used. One of them is artifical neural network (ANN) model and the other one is ensemble-learning method.

The basic concept of ANN comes from the way of biological neurons work. The ANN are composed of three layer classes like input layer, hidden layer and output layer as pictured in Figure 4.4. Input signals from an inlet layer are delivered to an outlet layer throughout hidden layers with aid of activation functions including the vectors of weight and bias. ANN links data of input with data of output via a series of nodes known as the interconnection of neurons. These connections are consist of some complex functions such as nonlinear functions. The weight factor of each input determines the interconnection strength. There are two ANN structure types according to the connections between their nodes such as the feedforward neural network (FFNN), and the feedback neural network (FBNN) or recurrent neural network (RNN). FFNN has one direction connection without backwards loop. Their signals proceed in the forward direction. In contrast to FFNN, FBNN or RNN has backward loop connection. Their signals proceed both forward and backward direction. The process of ANN modeling includes three steps: (1) data collecting and processing, (2) decision of model configuration, and (3) model training and confirmation [58-60].

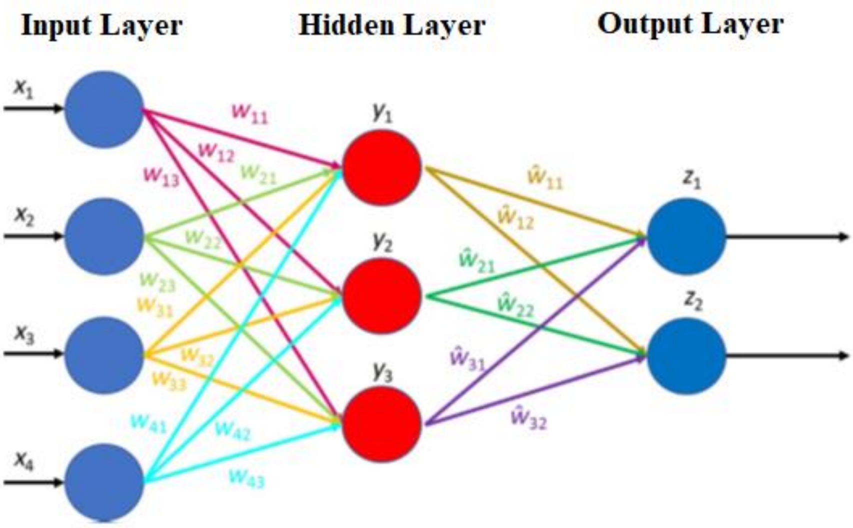


Figure 4.4: The structure of the ANN model (FFNN) [61].

Ensemble learning method trains several base learners as members of ensemble and aggregate their predictions in order to produce a single output. The structure of an ensemble learning is shown in Figure 4.5. The main target of ensemble learning is to improve accuracy of classification by combining estimations of multiple classifiers. Average (in the event of regression) and voting (in the event of classification) based predictions of each classifier are performed by ensemble learning. The final output being ensemble classifier has higher performance compared to any single classifier [62, 63].

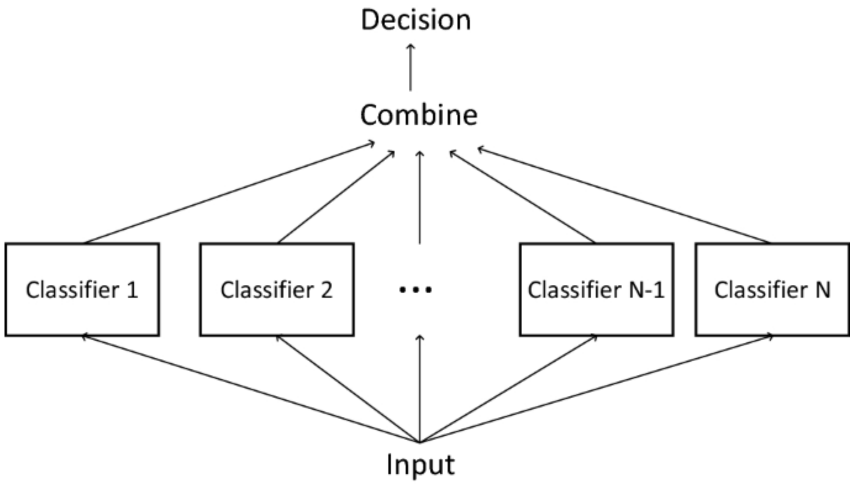


Figure 4.5: The structure of an ensemble learning [64].

4.1 Literature Review of Machine Learning about Exergy Analysis

Several studies indicated that ANN models are useful tools for exergy analysis. Azadbakht et al. applied the ANN model to estimate both energy and exergy variables of fluid bed dryer. While model inputs became temperature, speed and the beds depth, the model outputs became loss of exergy, energy usage and the ratio of energy usage. According to this study, a good overlap was observed between the estimated results and the measured results. The results of statistical analysis demonstrated that ANN could be applied for drying process having a large portion of energy utilization. Also, it was concluded that the prediction of a trained ANN is faster compared to mathematical models [65]. Since mechanistic models, which have complex processes consisting of the SLT efficiency are hard and time consuming, Osuolale and Zhang developed an ANN to model both exergy efficiency and compositions of product for systems of binary and multiple component in distillation columns. In addition, the ANN was used for optimization of exergy efficiency depending on quality constraint of product. According to this study, ANN models, which could be utilized to decide exergy efficiencies for various operational circumstances of distillation processes, provided excellent prediction result without complex calculation of the stream enthalpies and entropies. Also, proposed methods can enhance the distillation column exergy efficiency. As a result of the optimization, the methanol-water exergy efficiency increased by 11.2% and for benzene-toluene by 1.8%. In addition, modelling and optimization related with the models of ANN and BANN can help deciding of energy effective operations and distillation columns control [24].

In another research, the ANN model was developed for crude distillation column by Osuolale and Zhang. It was found that bootstrap aggregated neural network (BANN) models predict optimum working conditions of atmospheric distillation unit (ADU). Also, the result of BANN model gave accurate prediction. Considering this study, the neural network model can be created by using the historical data of plant. When a system is formed according to the actual operating conditions of a facility, the system can be continuously made better. The reason why using proposed system is because the recent operating conditions of plant can be utilized to train and set the ANN model. In addition, operators and engineers will have the opportunity to operate the facility in a very effective status thanks to the ANN model [66]. Osuolale and Anozie improved the optimization of ADU using ANN model based on exergy. Nine operation variables were used and optimization of ADU increased from 33% to 53% for exergy efficiency. The profiles of vapor and fluid exergy ratio in the fractionating column were used as a retrofit means to reveal inefficiency points inside the column and to propose possible column change options for energy efficient processes. It was observed that the exergy ratio profiles in the column intersected with each other. ADU's optimization enhanced the exergy efficiency from 53% to 60% provided that the intersection profiles of the exergy ratio of the column were eliminated.

The consequence of this study showed that the ANN is strong and suitable optimization model for solution of limited optimization problems like ADU with restricted operation variables [67]. Keçebaş et al. used the ANN modeling based on the algorithm of backpropagation learning to estimate the exergy performance of Afyonkarahisar geothermic district heating system (AGDHS) at a wide operational state ranges. The mean daily real thermic data obtained from AGDHS during the between 2009 and 2010 heating season was gathered as well as it is used to analyze exergy. The ANN prediction performance was evaluated using the coefficient of correlation; for instance, it can be mean relative and root mean square error. The ANN model presented good statistic behavior in general by a coefficient of determination known as R^2 in 0.9924-0.9942 interval, RMSs in the interval of 0.0571-0.0810, and 0.0020 for MARE. When the effects of input variables on some parameters such as flow velocity of heat exchanger output, environmental, well heat and outlet temperature were analyzed, the network gave reasonable results. According to results, the successful ANN model might be implemented to predict AGDHS's exergy efficiency with a good dependability and trueness [68].

The ANN model was built by Ghritlahre to estimate an exergy and energy efficiency of rough solar air heater with using the values of computed thermic and exergy efficiency and empirical thermic and exergy efficiency. The ANN model was trained using two learning algorithm. For the ANN model, the experiments time, flow rate of mass, intensity of solar radioactivity, environmental temperature, average air temperature and absorber layer temperature were considered as inputs; energy and exergy efficiency were evaluated as outputs. The effectiveness of ANN model was measured with using the analysis of statistical error. The determination coefficient values for exergy and energy efficiency are 0.95737 and 0.99921 respectively, which almost equal to one and hence give the correct results of the predictions. Considering the great accuracy achievement for the energy and exergy yieldance predictions of the solar air heater, multilayer perceptron ANN model can be preferred to examine energy and exergy yieldance of any solar power systems [69]. In a different study, Mohanraj et al estimated both exergy efficiency and destruction of direct extension solar-aided heat pump with building the ANN model relating to algorithm of backpropagation learning at various ambient circumstances. The consequences demonstrated that the network gave a maximal coefficient of correlation along with minimal variance coefficient and values of root mean square. In addition, the application of ANN model is quite feasible with reference to results [70]. Sadrameli and Alizadeh applied the modeling of ANN and generic algorithm (GA) combination to predict the total exergy performance of the olefin cracking furnaces located in Iran petrochemical plant. While steam ratio, residence time and coil outlet temperature were taken as input values, exergy efficiency was taken as output value in the combined ANN-GA model. The results indicated that the combination of ANN-GA model is very effectual method for optimizing the model performance and predicting the total exergy efficiency because correlation coefficient was obtained as 0.928 [71].

4.2 Modeling of the Vacuum Distillation Column Using ML Methods

The ML models might be applied to estimate exergy performance without difficulty of calculation both stream enthalpies and entropies. Also, this prediction can be used to decide whether the operation is efficient or not. The influences of various operational circumstances on the exergy performance of process can be evaluated on determining by the engineers and operators via this prediction tool. In this study, the predictive ability of ML models has been examined for different operational conditions on exergy efficiency of vacuum distillation column. Simulated process operational data of ASPEN HYSYS was used to both model input and output. Initially, the parameters that influence exergy efficiency were decided by way of "Case Study" of ASPEN HYSYS that generated the synthetic data. Considering the ML models, bootstrap aggregated neural network (BANN) and random forest models were used for prediction of exergy efficiency in R-Studio for this study. The data of both models are separated to training, testing as well as unseen validation data. This division is such that they are 50%, 30% and 20%, respectively. This neural network model for forecasting the exergy efficiency is given in equation 4.1:

$$\varphi = f(x_1, x_2, x_3) \tag{4.1}$$

Where φ is exergy efficiency, x_1, x_2, and x_3 are model input variables.

4.2.1 Bootstrap aggregated neural network

The neural network models could approximate any continuous nonlinear models but common neural networks may lack the ability of generalization when it is used to unseen data because of noise overfitting in the data [23]. Various techniques were proposed to develop the generalization ability of neural network such as regularization, Bayesian learning, early stopping, multiple network combination, training with static and dynamic process data. Among these techniques, the multiple network combination has an encouraging approach in respect to developing model estimation of unseen data. In addition, the accuracy of estimation about overall input space might be increased with using multi-neural network combination [72]. Breiman suggested a technique called as bootstrap aggregating, or bagging in 1996 [73]. Bootstrap aggregated neural network (BANN) is a resampling method that can be used to decrease the variance based on prediction with several classification and regression methods so develops the prediction of nonlinear models iteratively by using multiple models aggregation. It has a simple concept that shown in Figure 4.6: many samples of bootstrap are pulled from the present data, some prediction procedure is performed for each sample of bootstrap, and the outcomes are combined to get the total prediction. A chart of BANN is demonstrated in Figure 4.7.

In substitution for choosing a best accepted singular neural network model, they are put together to build a robust and accurate model. Total output of the BANN is obtained by weighted join of the singular neural network outputs. The BANN could be described with equation 4.2 [72, 73].

$$f(X) = \sum_{i=1}^{n} w_i f_i(X) \tag{4.2}$$

The aggregated neural network forecaster, the aggregating weight of i^{th} neural network combination, i^{th} neural network, neural networks number and the neural network inputs vector are indicated as $f(X)$, w_i, $f_i(X)$, n and X, respectively in equation 4.2.

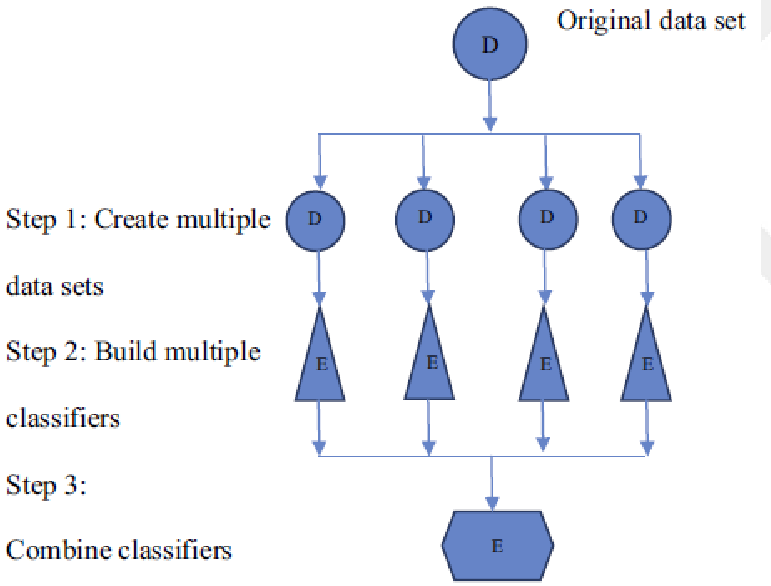


Figure 4.6: The concept of BANN [74].

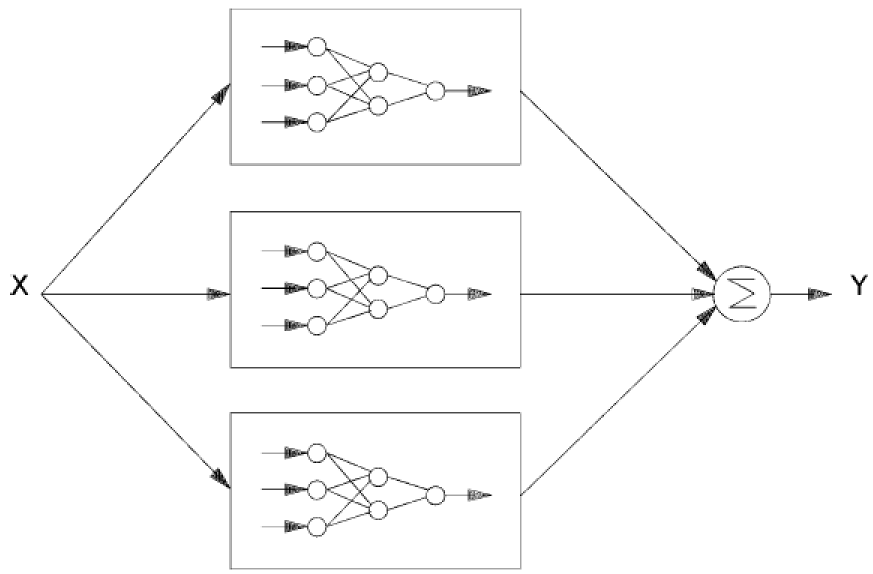


Figure 4.7: Bootstrap aggregated neural network [24, 72].

4.2.2 Random forest

Leo Breiman and Adele Cutler combined the methods of “bootstrap aggregating” and “random subspace” to develop random forest (RF) creating a group of decision trees and classifying them. The RF, which is a robust ML algorithm, is an ensemble learning method for performing tasks such as regression and classifications. The RF benefits from bagging approach. The RF incorporates the classifiers of multiple decision tree and the result categories are decided according to the status of decision tree classification outputs like Figure 4.8. RF algorithms have three major parameters that have to be adjusted before training. These involve the size of node, the trees number, and the number of sampled features. For building one decision tree, the RF algorithm uses two processes of random selection. Firstly, random training samples are selected. The sample of arbitrary dataset is trained with several times to get a prediction model. The RF works through improving a large number of decision trees at time of training. Secondly, the random characteristics qualities of the sample are selected and the RF gives the mode output (classification) of classes or the average estimation (regression) of individual trees. After whole decision trees are created, the ending classification result is decided by the voting method of equal weight. The broad datasets are handled without loss of dimensionality by the RF. Getting the sum of multiple decision trees will provide better performance, even if it is sensitive to overfitting. Also, the importance measurement of the predictor variables is helpful in terms of interpreting the RF model and the selecting of variable [57, 59, 75-77].

The RF model is preferred from a computer viewpoint in terms of some features that are listed below [77]:

- Handling of both classification and regression
- Dependence of very few tuning parameters
- Fast training and prediction relatively
- Having an inbuilt estimation of generality error
- Applicable in parallel
- Option to be used in high dimensional problems

The RF model is preferred statistically in terms of extra features that are listed below [77]:

- Measurement of variable importance
- Detection of outlier
- Imputation of missing value
- Differential class weight
- Visualization
- Unsupervised learning

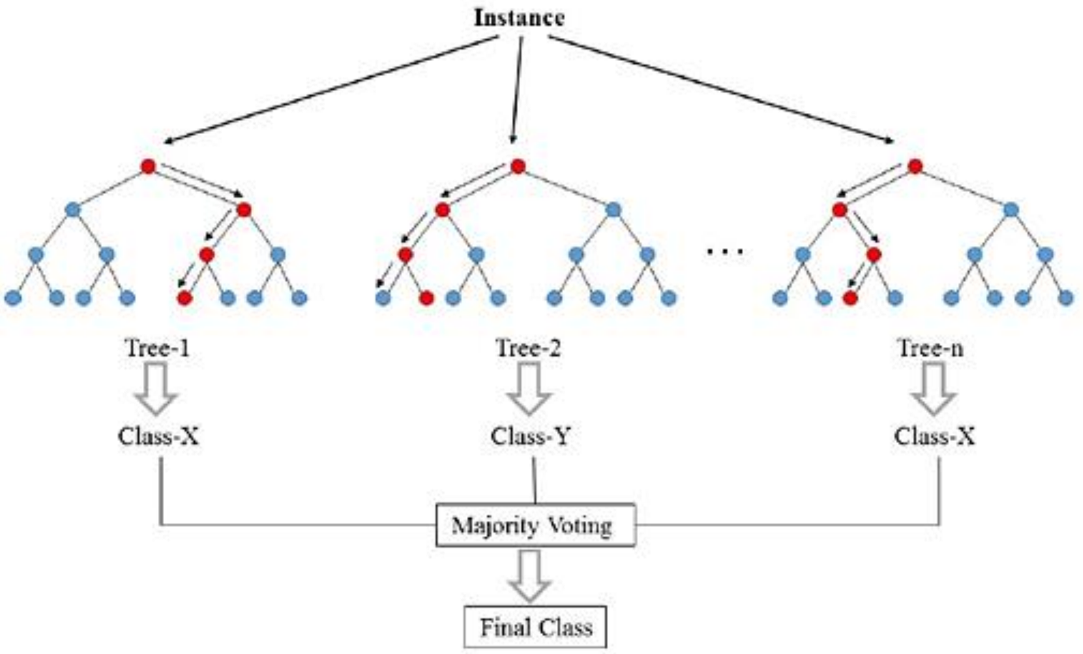


Figure 4.8: Diagram of the RF classifier [78].

5. RESULTS AND DISCUSSIONS

5.1 Comparison of Simulation Results with Real Values

Comparison of the simulation results with the actual values is important before exergy and energy studies in terms of accuracy of calculation results. For this reason, all real operation values such as temperature, pressure, flow were compared with simulation results. Exergy and energy calculations were made after the simulation results converged to real values as much as possible. Table 5.1 indicates the comparison between simulation and actual values of column tray temperatures in reference to absolute difference and relative error.

Table 5.1: Comparison between simulation and actual values of column tray temperatures.

Tray	Absolute Difference	Relative Error %
1	0.000	0.000
2		
3	0.205	0.174
4		
5		
6		
7		
8		
9	2.256	0.924
10		
11	2.543	0.820
12		
13	2.008	0.692
14		
15		

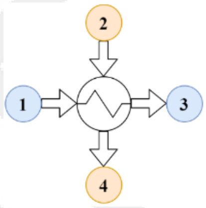
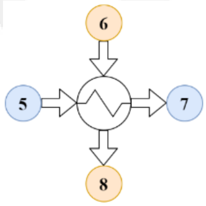
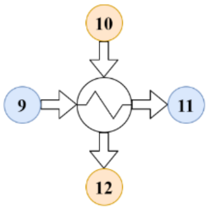
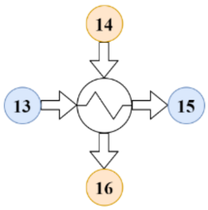
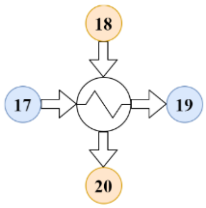
Also, comparison based on the absolute difference and relative error of column return temperatures with real and simulation values is given in Table 5.2.

Table 5.2: Comparison of column return temperatures with real and simulation values.

	Return Temperature (°C)	
PA Type	**Absolute Difference**	**Relative Error %**
PA1	0.0543	0.1713
PA2	0.0184	0.0319
PA3	0.1004	0.0509
PA4	0.3809	0.1423
PA5	0.0037	0.0012

In addition, comparisons between simulation and actual values were made for some heat exchangers that based on the absolute difference and relative error in Table 5.3.

Table 5.3: Comparisons between simulation and actual values were made for some heat exchangers.

	Stream No.	Absolute Difference	Relative Error (%)	Symbolic HE
E1	1	0.000	0.000	
	2	0.203	0.086	
	3	2.513	1.209	
	4	1.514	1.654	
E2	5	0.084	0.047	
	6	0.055	0.022	
	7	3.954	1.956	
	8	1.628	0.898	
E3	9	0.008	0.004	
	10	0.297	0.096	
	11	1.028	0.387	
	12	0.077	0.031	
E4	13	0.032	0.016	
	14	0.006	0.002	
	15	2.657	1.042	
	16	0.236	0.110	
E5	17	0.007	0.003	
	18	0.041	0.012	
	19	1.703	0.566	
	20	2.512	0.842	

Consequently, very close results were achieved by comparison with simulation and actual values as sighted in Table 5.1, Table 5.2 and Table 5.3. At the same time, all these comparisons were made in all unit operations of the plant for all operation values.

5.2 Energy and Exergy Analysis of All Unit Operations

The flowchart shown in Figure 5.1 was used to carry out calculations of exergy and energy analysis for every single unit operations in ASPEN HYSYS. The necessary data such as equipment design, laboratory and operation values was obtained for simulating the VDU. Then, simulation results were compared with the actual values. When the simulation results are appropriate, energy and exergy analysis was performed for every single unit operations by using the required equations in section three. Necessary simulation outputs of each stream are used in order to use these equations calculating energy and exergy.

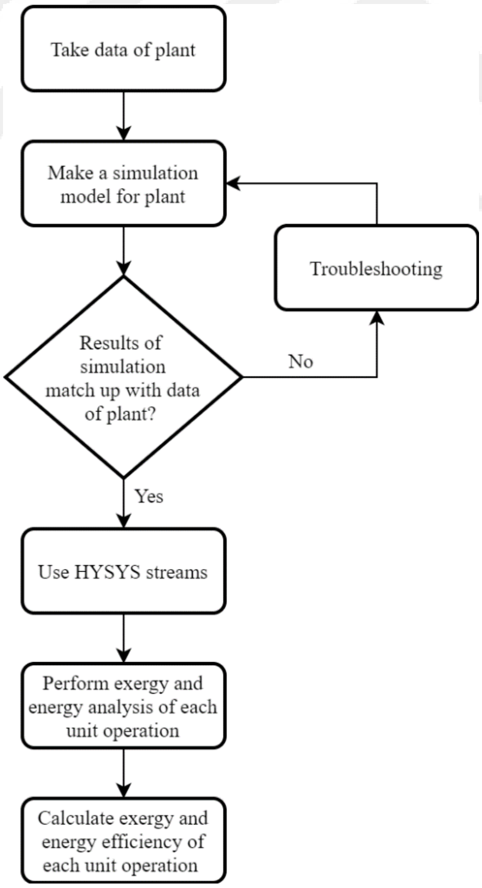


Figure 5.1: The flowchart of energy and exergy calculation for all unit operations in ASPEN HYSYS.

Selection of exergy transfer method is important for exergy calculation. Equations 3.17, 3.19 and 3.20 are used for each transfer method. After input and output exergy calculation is done, exergy efficiency calculation is applied by using equation 3.22. In addition, energy efficiency is calculated equation 3.21. The loss of exergy that is named irreversibility is done by using equation 3.29. Also, Table 3.2 is used to calculate exergy efficiency and loss for each unit operation. Both energy and exergy calculations of each unit operations are done by creating spreadsheets in ASPEN HYSYS.

5.2.1 Energy and exergy calculation of a heat exchanger

Table 5.4 shows the calculation results of exergy and energy for E1 heat exchanger of VDU. Irreversibility calculation of E1-1 is given by equation 5.1. Also, equation 5.1 can be expressed as equation 5.2 that is the difference of the summation of exergy input rate and the summation of exergy output rate.

$$\dot{I}_{E1-1} = \dot{m}_1(ex_1 - ex_3) + \dot{m}_2(ex_2 - ex_4) \tag{5.1}$$

$$\dot{I}_{E1-1} = (\dot{m}_1 ex_1 + \dot{m}_2 ex_2) - (\dot{m}_1 ex_3 + \dot{m}_2 ex_4) \tag{5.2}$$

Where the sum of exergy input and output rate for the E1-1 is given by equation 5.3 and 5.4 respectively.

$$\sum_i \dot{E}x_i = \dot{m}_1 ex_1 + \dot{m}_2 ex_2 \tag{5.3}$$

$$\sum_o \dot{E}x_o = \dot{m}_1 ex_3 + \dot{m}_2 ex_4 \tag{5.4}$$

Exergy efficiency of E1-1 heat exchanger is calculated according to equation 5.5 in Table 3.2.

$$\psi_{E1-1} = {\dot{E}x_{cold,o} - \dot{E}x_{cold,i}} \Big/ {\dot{E}x_{hot,i} - \dot{E}x_{hot,o}} \tag{5.5}$$

Moreover, equation 5.5 corresponds to equation 5.6.

$$\psi_{E1-1} = (\dot{m}_1 ex_3 - \dot{m}_1 ex_1) \Big/ (\dot{m}_2 ex_2 - \dot{m}_2 ex_4) \tag{5.6}$$

Table 5.4: Exergy and energy calculations for E1 heat exchanger.

E1-1	H_{in} (kj/s)	H_{out} (kj/s)	Q (kj/s)	Exergy Rate (kj/s)	I (kj/s)	Energy Efficiency	Exergy Efficiency
In (1)	-62384.1994			586.8611			
In (2)	-57368.5349			1673.5318			
Out (3)		-60672.4068		1146.6473			
Out (4)		-59080.3275		933.9857			
	-119752.7343	-119752.7343	0.0000		179.7598	1.0000	0.7569
E1-2	**H_{in} (kj/s)**	**H_{out} (kj/s)**	**Q (kj/s)**	**Exergy Rate (kj/s)**	**I (kj/s)**	**Energy Eff**	**Exergy Eff**
In (5)	-60995.1932			1025.6604			
In (6)	-55152.3595			2887.4090			
Out (7)		-58779.0177		2000.7221			
Out (8)		-57368.5349		1673.5318			
	-116147.5526	-116147.5526	0.0000		238.8155	1.0000	0.8033
E1-3	**H_{in} (kj/s)**	**H_{out} (kj/s)**	**Q (kj/s)**	**Exergy Rate (kj/s)**	**I (kj/s)**	**Energy Eff**	**Exergy Eff**
In (9)	-58676.5153			2052.7199			
In (10)	-49264.5649			7168.4324			
Out (11)		-52788.7208		5881.9468			
Out (12)		-55152.3595		2887.4090			
	-107941.0802	-107941.0802	0.0000		451.7966	1.0000	0.8945

Exergy calculations can be done by using standard enthalpy and entropy values instead of exergy directly given by ASPEN HYSYS. Between equation 5.7 and 5.10 gives exergy rate of each stream for E1-1. Exergy efficiency calculations can be done with using these exergy rate equations.

$$\dot{E}x_1 = \dot{m}_1[(h_1 - h_o) - T_o(s_1 - s_o)] \tag{5.7}$$

$$\dot{E}x_2 = \dot{m}_2[(h_2 - h_o) - T_o(s_2 - s_o)] \tag{5.8}$$

$$\dot{E}x_3 = \dot{m}_3[(h_3 - h_o) - T_o(s_3 - s_o)] \tag{5.9}$$

$$\dot{E}x_4 = \dot{m}_4[(h_4 - h_o) - T_o(s_4 - s_o)] \tag{5.10}$$

5.2.2 Energy and exergy calculation of a furnace or heater

For this study, the furnace of VDU was simulated as a heater in ASPEN HYSYS. Equation 5.11 gives the exergy efficiency of furnace. Detailed energy and exergy calculations of furnace are stated in Table 5.5.

$$\psi_{furnace} = \dot{m}_{13}(ex_{13} - ex_{14}) / \dot{Q} = Ex_{13} - Ex_{14} / \dot{Q} \tag{5.11}$$

Table 5.5: Exergy and energy calculations for furnace.

Furnace	Inlet Stream	Outlet Stream
	(13)	**(14)**
Exergy (kj/s)	20324.9432	37993.3390
I (kj/s)	-17668.3959	
H (kj/s)	-160260.4355	-126128.1394
Q (kj/s)	-34132.2961	
Energy Efficiency	0.7870	
Exergy Efficiency	0.5176	

5.2.3 Energy and exergy calculation of a pump

Exergy efficiency for G-2 pump is calculated by equation 5.12 or 5.13. In addition, both energy and exergy calculations are given Table 5.6.

$$\psi_{G-2} = [\dot{m}_{15}(ex_{15} - ex_{16})] / [\dot{m}_{15}(h_{15} - h_{16})] \tag{5.12}$$

$$\psi_{G-2} = 1 - {}^{(T_0 S_{gen,G-2})}\!\Big/_{(H_{16} - H_{15})} \tag{5.13}$$

Where the generation of entropy, $S_{gen,G-2}$, for the G-2 pump is given by equation 5.14.

$$S_{gen,G-2} = \dot{m}_{15}(s_{16} - s_{15}) = S_{16} - S_{15} \tag{5.14}$$

In addition, exergy loss can be calculated with equation 5.15.

$$I_{G-2} = T_0 S_{gen,G-2} \tag{5.15}$$

Table 5.6: Exergy and energy calculations for G-2 pump.

G-2	**Inlet Stream**	**Outlet Stream**
	(15)	**(16)**
Exergy (kj/s)	20042.8152	20075.1561
I (kj/s)	13.5389	
H (kj/s)	-106647.9642	-106602.0845
S (kj/s-C)	284.3775	284.4229
Q (kj/s)	-45.8797	
Energy Efficiency	0.9996	
Exergy Efficiency	0.7049	

5.2.4 Energy and exergy calculation of a vacuum distillation column

Energy and exergy calculations for the vacuum distillation column are shown in Table 5.7. Exergy efficiency calculation can be done using either equation 5.16 or equation 5.17.

$$\psi_{VDU} = {}^{\sum_o \dot{E}x_o}\!\Big/_{\sum_i \dot{E}x_i} \tag{5.16}$$

$$\psi_{VDU} = {}^{[\sum_i \dot{E}x_i + \dot{E}x_Q - \dot{I}_{VDU}]}\!\Big/_{\sum_i \dot{E}x_i} \tag{5.17}$$

The necessary expressions such as the rate of exergy input and output, exergy destruction, as well as heat exergy for equations 5.16 and 5.17 are calculated from the following equations.

$$\sum_i \dot{E}x_i = \dot{m}_{17}ex_{17} + \dot{m}_{18}ex_{18} + \dot{m}_{19}ex_{19} \tag{5.18}$$

$$\sum_{o} \dot{E}x_o = \dot{m}_{20}ex_{20} + \dot{m}_{21}ex_{21} + \dot{m}_{22}ex_{22} + \dot{m}_{23}ex_{23} + \dot{m}_{24}ex_{24} + \dot{m}_{25}ex_{25} \tag{5.19}$$

$$\dot{E}x_Q = (1 - {T_0}/{T})\dot{Q}_{VDU} \tag{5.20}$$

$$\dot{I}_{VDU} = \sum_{i} \dot{E}x_i - \sum_{o} \dot{E}x_o + \dot{E}x_Q \tag{5.21}$$

Where the expressions of equation 5.18 to 5.21 are exergy inlet rate, exergy exit rate, heat exergy and exergy destruction, respectively.

After doing the exergy and energy calculations for each unit operations of the plant, Figure 5.2 showing the both exergy and energy efficiency of unit operations is obtained. It is seen that almost all of the energy efficiency results are equal to one, except for the column and the furnace. At the same time, the energy efficiency of the column was greater than one. This proves that the energy efficiency calculation can be insufficient and incorrect in determining the losses.

According to Figure 5.3, the E-12 heat exchanger using cooling water has the lowest exergy efficiency due to heat released through hot water into the environment and bypass flow on the cooling waterside. At the same time, the performance of the E-12 heat exchanger may decreased due to the contamination on the waterside. Another low exergy efficiency equipment among all unit operations is the furnace with 0.518 exergy efficiency. Moreover, Izyan and Shuhaimi conducted the exergy analysis on crude preheat train and furnace taking part a crude distillation unit. They found that the furnace has the highest exergy destruction with 86% of overall exergy destruction in the system [22]. Waheed et al. performed thermodynamic analysis of a petroleum distillation unit to specify inefficiencies and they found that the most inefficient equipment were the furnaces responsible for 51.6% of all exergy destructions [55]. There is a decrease in the efficiency of the furnace due to unwanted heat losses. They can be caused by loss of heat to the environment from the exterior surface of the walls via radiation and convection, loss of heat via exhaust gases, loss of heat via furnace walls as well as loss of heat via gases leaking from clefts, openings [79]. Therefore, low exergy efficiency due to unwanted losses in the furnace, which is a high energy intensive process, is an expected result.

The E-13 is an air cooler that also has the low exergy efficiency with 0.62. Exergy efficiency of an air cooler is expected to be low due to the high temperature drop and the heat released through hot air into the environment so these situations cause exergy loss. Vilarinho et al. carried out energy and exergy study in the pre-distillation unit. It was concluded that air coolers are one of the lowest efficient equipment in the unit, with an energy loss of 59.9% and an exergy loss of 11.2%. They also found that the greatest exergy loss was in the furnace with 56.3% [21].

Vacuum distillation column with an exergy efficiency of 0.657 follows the E-13 air cooler in Figure 5.3. Exergy loss of column occurs with entropy generation arising from irreversibility. Exergy loss can be measured by the irreversibility occurring in the column because of the loss of momentum, thermal as well as chemical potential that can be also called as driving force of pressure, temperature and mass, respectively. Column entropy increases with the mass and heat transfer occurring between flows. In addition, condenser entropy increases with the just heat transfer. Also, mixing during separation process causes the irreversibility. Moreover, the total exergy efficiency of the column consists of the exterior and interior exergy efficiencies. Thermal integration between units, overhead stream coproduction and recompression for the reboiler are related to exterior exergy efficiency. However, column interior design, column stage number, composition and position of feed as well as utility demand are related to interior exergy efficiencies. Many distillation columns have low exergy efficiency in the range of 20-25%, whereas specified modifications can enhance the exergy efficiency by up to 60% [80, 81]. Odejobi applied an exergy analysis in a petroleum distillation unit. It was concluded that among the other equipment, both maximum irreversibility and minimum exergy efficiency of 52.1% occurred in the column [82]. Accordingly, when compared to the general average exergy efficiency of the columns, it is understood that the vacuum distillation column has a very high exergy efficiency of 0.657.

Generally, it is seen that the exergy efficiencies of the heat exchangers between E-1 and E-11 are high with the range of 0.792-0.937 in Figure 5.2. Among the preheat train, the performance of E-1 is lower since it depends on the bypass flow condition. The exergy efficiency of the pumps also varies between 0.705 and 0.877 in Figure 5.2. Since G-2 is a vacuum bottom pump, it is normal for its performance to be lower than other pumps.

Table 5.7: Exergy and energy calculations a vacuum distillation column.

VDU	Inlet Streams (17-19)			Outlet Streams (20-25)					
	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)	(25)
Exergy (kj/s)	37993.3390	1538.2114	0.0000	-10.2675	246.6981	4332.2077	4674.0268	4073.8481	12649.7015
ΣExergy	39531.5504			25966.2147					
I (kj/s)	8562.3746								
H (kj/s)	-126128.1394	-43739.8034	0.0000	-3860.0002	-18490.9885	-56233.9684	-34344.3975	-21516.2704	-60162.0334
ΣH	-169867.9427			-194607.6585					
Q (kj/s)	24739.7157								
Energy Eff.	1.1456								
Exergy Eff.	0.6568								

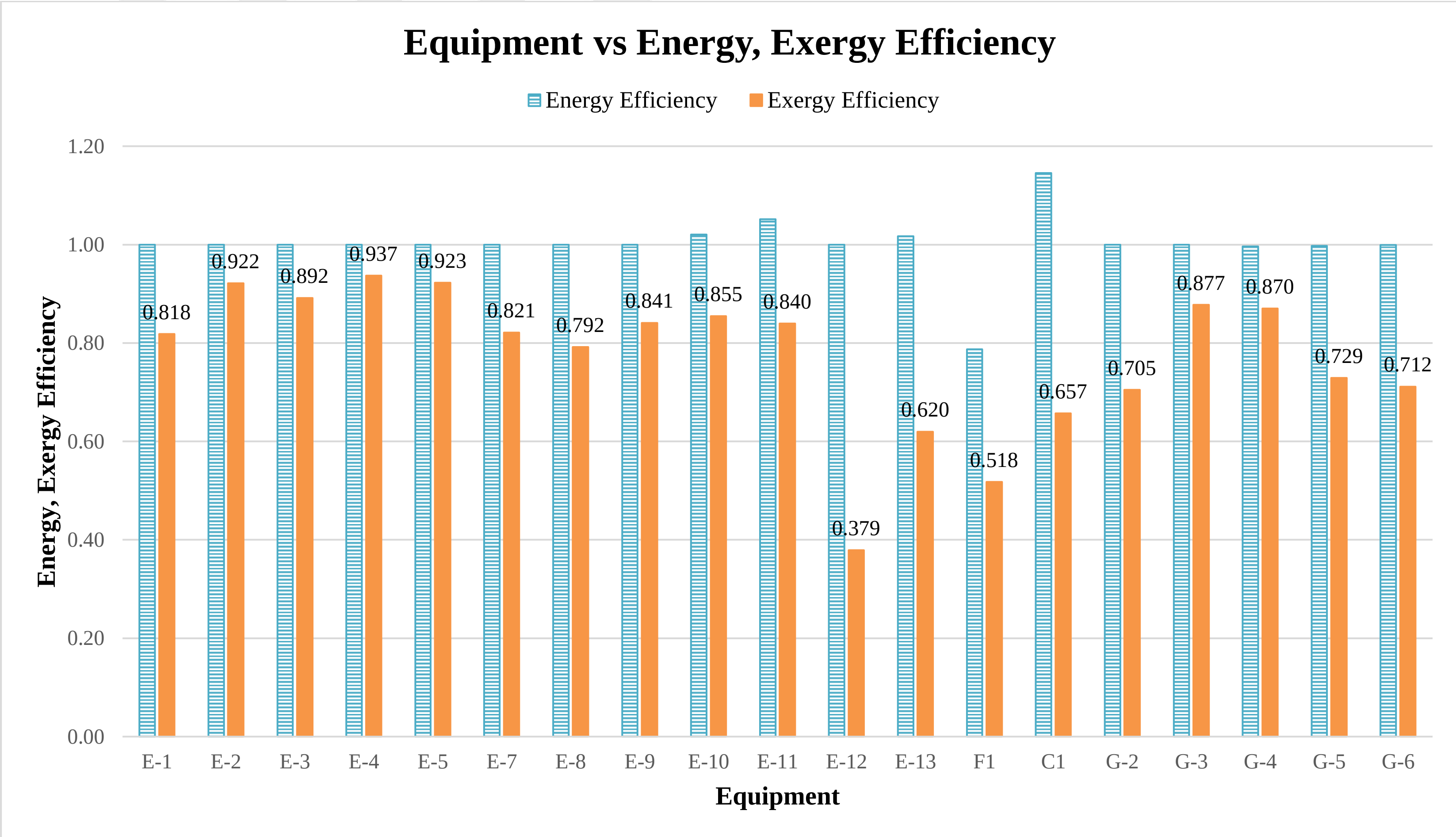


Figure 5.2: The exergy and energy efficiencies of all unit operations in the plant.

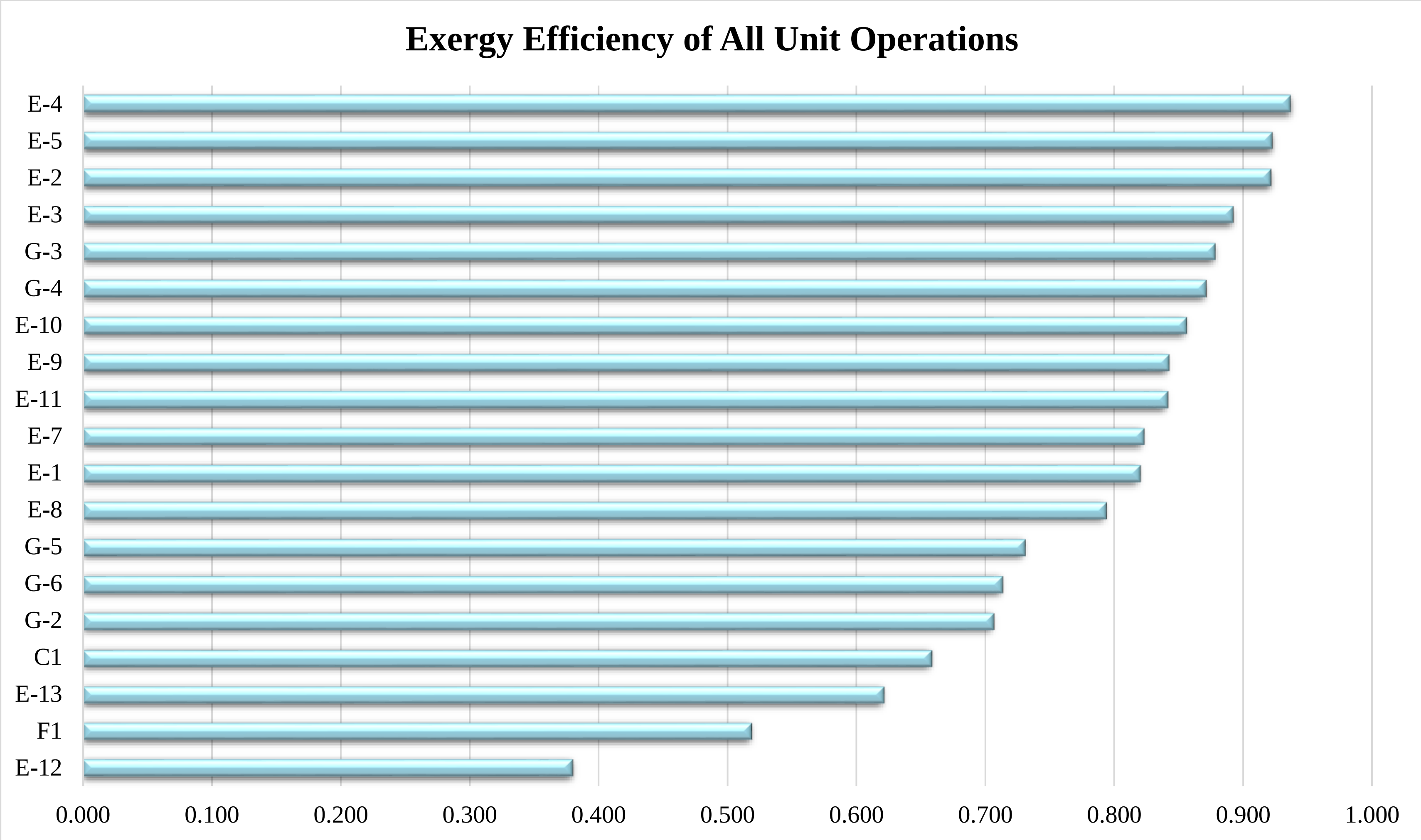


Figure 5.3: Listing the magnitude of exergy efficiencies for all unit operations.

5.3 Exergy Study in Vacuum Distillation Column with Using Machine Learning

There are many process control limits in the vacuum distillation column. Using these limits, a case study was conducted in ASPEN HYSYS. This case study investigates the change in exergy and energy efficiency for lower and upper limits range of the process control variables in the vacuum distillation column. Not only the process control limits but also the effect of the furnace exit temperature on the column exergy and energy efficiency was examined. These consequences are given in Table 5.8.

Table 5.8: The effect of operating parameters on exergy efficiencies of the column.

Operating Parameters	Exergy Efficiency Change	% Absolute Exergy Change	Energy Efficiency Change	% Absolute Energy Change
PA1 flow (t/h)	0.6499-0.6576	1.185	1.138-1.131	0.615
PA2 flow (t/h)	0.6552-0.6567	0.229	1.133-1.132	0.088
PA2 temperature (°C)	0.6570-0.6560	0.152	1.132-1.133	0.088
PA3 flow (t/h)	0.6565-0.6536	0.442	1.133-1.134	0.088
PA3 temperature (°C)	0.6431-0.6560	2.006	1.138-1.133	0.439
PA4 flow (t/h)	0.6555-0.6599	0.671	1.133-1.131	0.177
PA4 temperature (°C)	0.6571-0.6442	1.963	1.132-1.138	0.53
PA5 flow (t/h)	0.6560-0.6556	0.061	1.133-1.133	0
PA5 temperature (°C)	0.6529-0.6560	0.475	1.134-1.133	0.088
PA6 temperature (°C)	0.6560-0.6560	0	1.133-1.133	0
Furnace exit temperature (°C)	0.6655-0.6290	5.485	1.124-1.157	2.936

According to results of Table 5.8, the operating parameters of vacuum distillation column's pump-arounds such as flow and temperature do not have a considerable effect on the column exergy efficiency. Among these operating parameters shown in Table 5.8, three parameters most affect the exergy performance of the vacuum distillation column. The most affecting factors on the column exergy efficiency are respectively furnace exit temperature, PA3 temperature and PA4 temperature. Dincer and Rosen examined the effect of operational parameters such as temperature and pressure on the exergy and energy efficiency of the vacuum distillation column. They found that the impact of these operational changes on the both exergy and energy efficiency was only in the 2% range. They concluded that the exergy and energy yieldances of the vacuum distillation column were almost never affected by these operational changes [20].

5.4 Exergy Study in Vacuum Distillation Column with Using Machine Learning

In this study, the BANN and the RF models were developed for exergy predictions according to the most affecting parameters on vacuum distillation column such as furnace exit temperature as well as PA3 and PA4 temperature, which are the model inputs. Figure 5.4 and Figure 5.6 shows the scatter plots of the BANN and RF model predicted versus actual column exergy efficiency on training, testing and validation datasets, respectively. When the plots are examined, it is seen that the actual outcomes are close to the predicted values. The accuracy of the model increases if all points are closer to the diagonal line. In addition, it is realized that the datasets of BANN model graph in Figure 5.4 is more scattered than the RF model in Figure 5.6. Therefore, this result gives that the RF model can predict to column exergy efficiency more accurately. Figure 5.5 and Figure 5.7 demonstrate the BANN and RF model performances in prediction of column exergy efficiency for training, testing and validation datasets, respectively. Red dashed lines represent the actual values while blue lines represent predicted values in Figure 5.5 and Figure 5.7. It can be seen that the BANN and RF model prediction results in Figure 5.5 and Figure 5.7 are fitted with the actual values. However, when Figure 5.5 and Figure 5.7 are compared, it is seen that the predicted values of the RF model overlap the actual values better, so it gives more accurate prediction results. The decreasing trend in Figure 5.5 and Figure 5.7 is due to the furnace exit temperature, which is one of the model inputs. As the furnace exit temperature increases, the column input flow exergy increases and consequently the exergy efficiency of the column decreases. In the RF model, Figure 5.8 showing the order of importance variables for training, testing and validation datasets can be obtained. The RF model uses two calculation methods for this, namely Mean Decrease Accuracy (%IncMSE) and Mean Decrease Gini (IncNodePurity). According to Figure 5.8, the most important factor affecting column exergy efficiency is the furnace exit temperature. Also, there are various statistical methods for evaluating the model performances. The mean squared error (MSE) was used for this study. In Table 5.9, it is seen that the mean squared error of the RF model is lower than the BANN model, so it was proved that the RF model predicts exergy efficiency better by the MSE method. All in all, it was concluded that exergy efficiency can be predicted with ML models without performing complex exergy calculations.

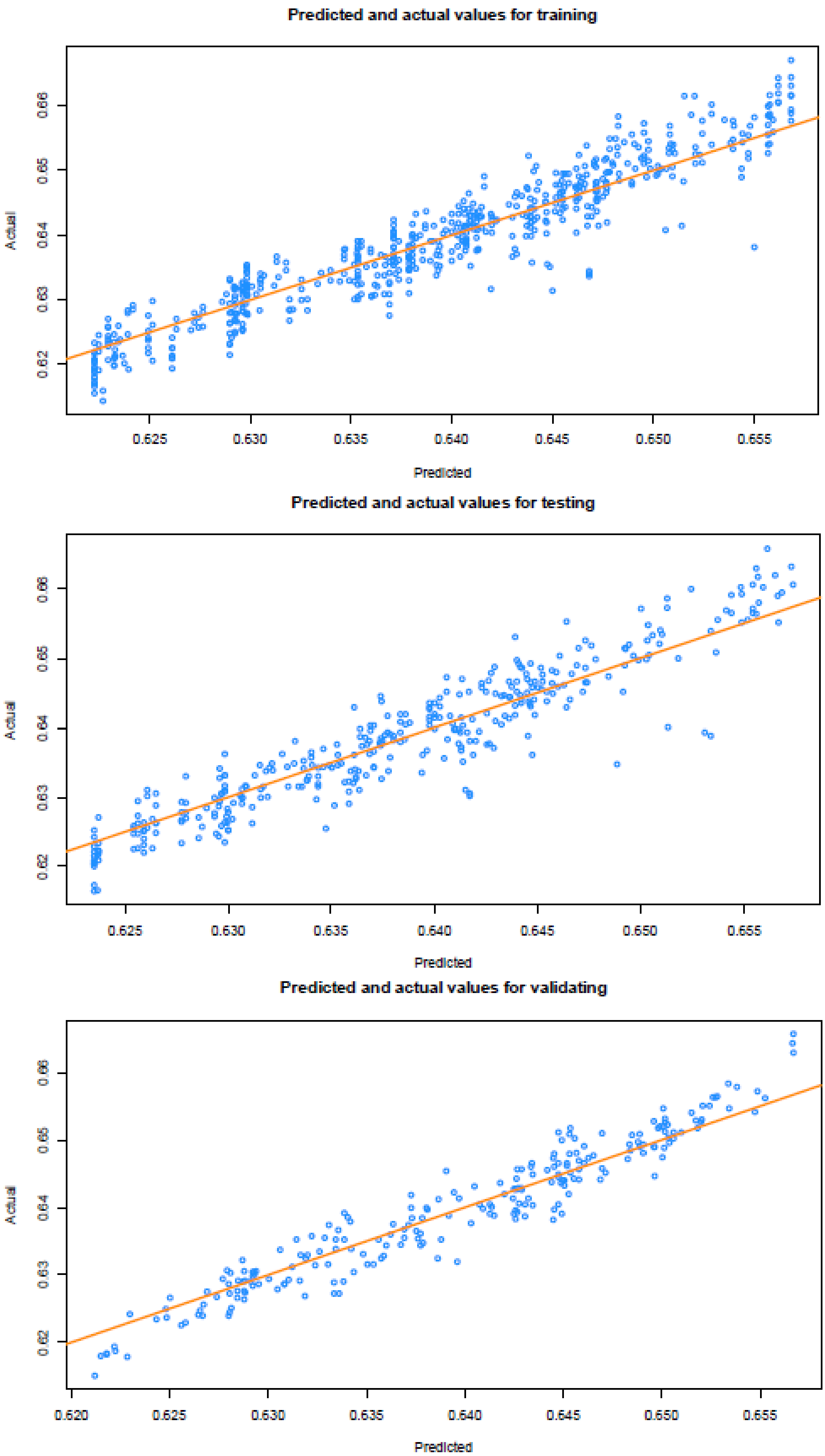


Figure 5.4: Scatter plot of the BANN model predicted versus actual exergy efficiency of the column for training, testing and validating data.

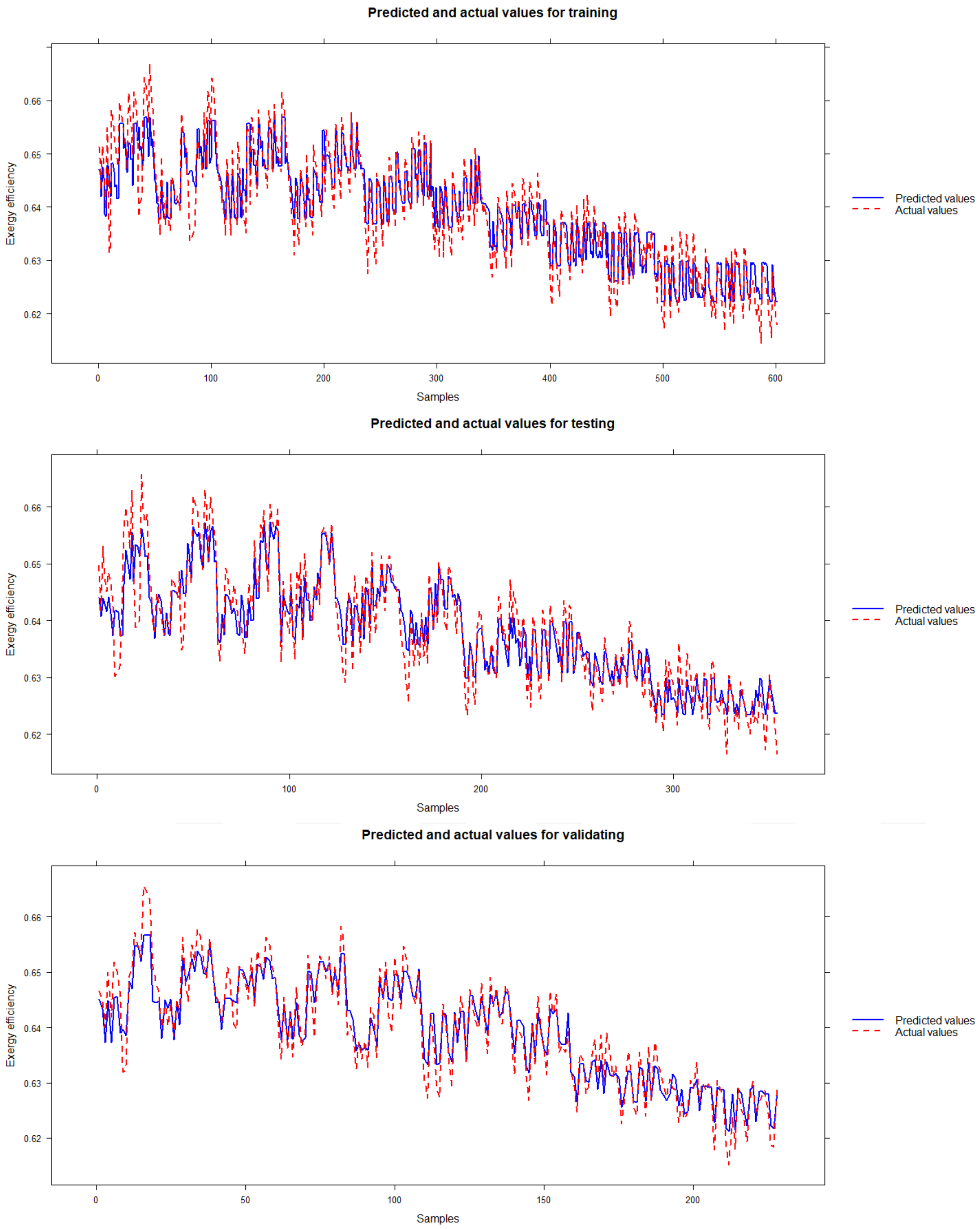


Figure 5.5: The BANN model predicted and actual exergy efficiency of the column for training, testing and validating data.

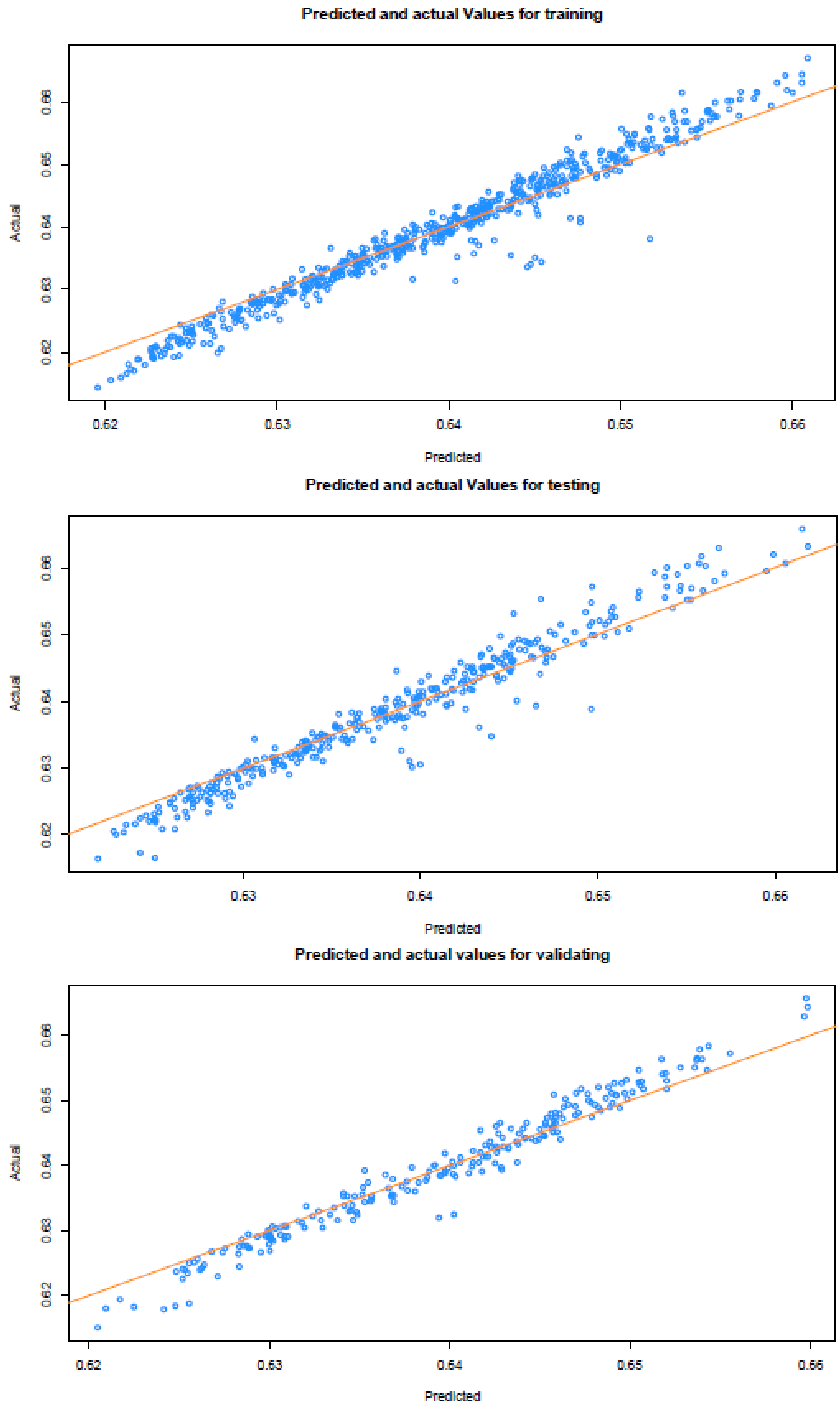


Figure 5.6: Scatter plot of the RF model predicted versus actual exergy efficiency of the column for training, testing and validating data.

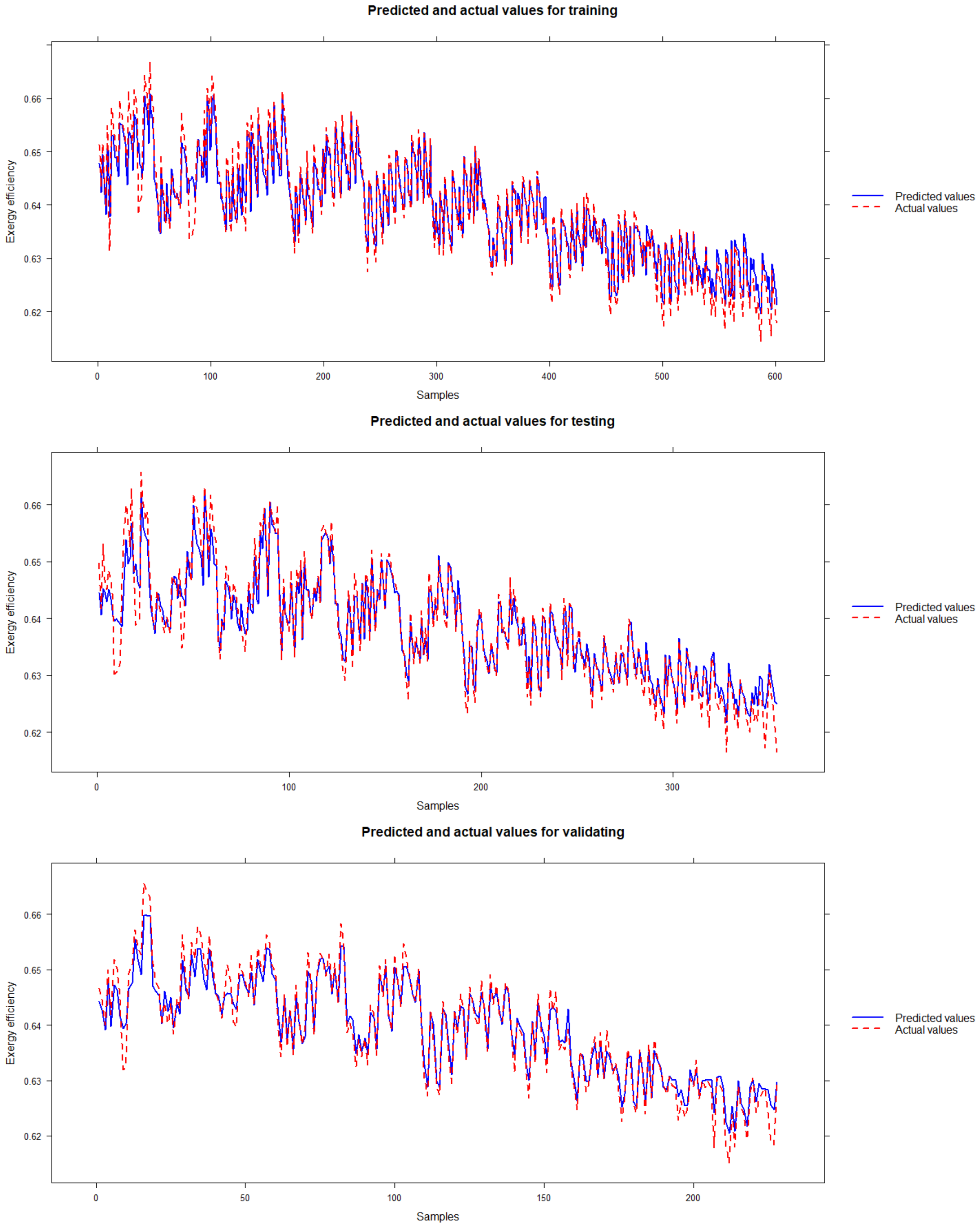


Figure 5.7: The RF model predicted and actual exergy efficiency of the column for training, testing and validating data.

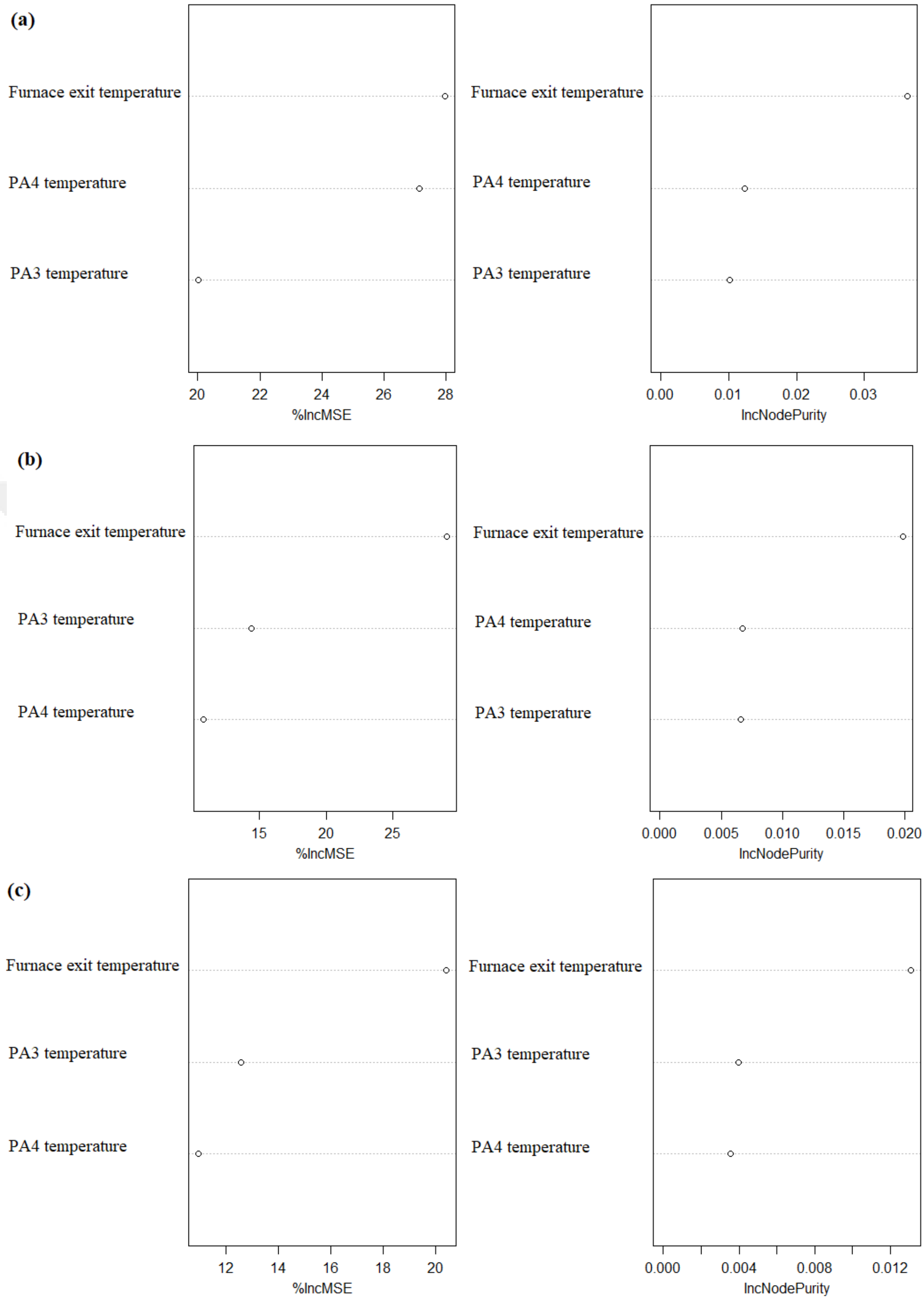


Figure 5.8: Variable importance for (a) training (b) testing (c) validating data.

Table 5.9: Evaluating model performance with Mean Squared Error.

	Training	**Testing**	**Validation**
BANN model	0.0000126	0.0000132	0.0000080
RF model	0.0000060	0.0000064	0.0000047

6. CONCLUSION

In this study, the exergy and energy investigation of the vacuum distillation unit in TUPRAS Refinery was performed. The formulations required to perform exergy and energy calculations were found through literature research. After collecting all the data required for simulation, the unit was simulated with ASPEN HYSYS. Each equipment in the VDU was evaluated in both energy and exergy studies. An additional study was carried out for the exergy efficiency of the column. By using the limit values of the process control parameters affecting the column, the effect of operational parameters on the column exergy efficiency was examined with the case study feature of ASPEN HYSYS. After deciding on the parameters affecting the column, the exergy efficiency prediction in the column was studied with machine learning models.

The results achieved in this study are listed below.

1. Simulation is an important tool in exergy and energy calculations, evaluating results, and applying various case studies.
2. Exergy and energy analysis results are compared for each unit operation. While losses can be seen in exergy calculations, these losses cannot be seen in energy calculations. Therefore, energy efficiency calculations are insufficient in the performance evaluation of the unit operations. Instead of energy, exergy is a powerful tool in determining performance decrease of the unit operations.
3. When exergy efficiency results are examined for each equipment, the lowest five equipment are E-12 heat exchanger using cooling water, furnace, E-13 air cooler, vacuum distillation column and G-2 pump that have the exergy efficiency of 0.379, 0.518, 0.620, 0.657 and 0.705, respectively. In the cooling heat exchangers and air coolers, exergy efficiency decreases due to reasons such as high temperature drop and heat released to the environment. The furnace is an energy-intensive equipment and a decrease in exergy efficiency is common due to unwanted heat losses. Although the column is on the list of low exergy efficiency, it actually has a very high efficiency compared to

general column efficiencies in the literature. The reason for the low performance of G-2 among pumps is that it is a vacuum bottom pump.

4. When all operational parameters such as PA temperature and flow affecting the column were evaluated, it was understood that these parameters did not significantly affect the column exergy efficiency. Except for the furnace exit temperature, only 2% exergy efficiency change was observed. Therefore, it was understood that there was very little operability part in the column in order to increase energy efficiency. The main parameters affecting the column were the furnace exit temperature, PA3 and PA4 temperatures, respectively.
5. The BANN and RF ML models were used to estimate the column exergy efficiency. It has been found that they are successful in predicting exergy efficiency. Good overlap was observed between the actual values and the model predicted values on training, testing and validation data. These results were also supported by MSE. It was observed that the RF model has a higher prediction performance compared to the BANN model.
6. The predictability of exergy efficiency in the column was proven without the need for ASPEN HYSYS simulation study and complex exergy calculations. At the same time, using these prediction models, it can be decided for which operational conditions the column is efficient or not.

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