

Design of Cryogenic Distillation Column for hydrogen isotope separation

A PROJECT REPORT

Submitted by
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DECLARATION BY THE SCHOLAR

I hereby declare that this submission is my own and that, to the best of my knowledge and belief, it contains no material previously published or written by another person nor material which has been accepted for the award of any other Degree or Diploma of the University or other Institute of Higher learning, except where due acknowledgement has been made in the text.

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CERTIFICATE

This is to certify that the thesis entitled “**DESIGN OF CRYOGENIC DISTILLATION COLUMN FOR HYDROGEN ISOTOPE SEPARATION**” submitted by **AISHWARYA VINAY KUMAR (R670215004)**, to the University of Petroleum and Energy Studies, for the award of the degree of Master of Technology in Chemical Engineering with specialization in Process Design Engineering is a bonafide record of project work carried out by her under our supervision. The results embodied in this project report are based on literature and the research done in Institute for Plasma Research.

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Abstract

Cryogenic distillation is preferred to other methods of gas separation at industrial scale because it has the advantage of high separation factors, the possibility to process large amounts of gas while obtaining high purity gases. Similar with the conventional distillation processes, separation by cryogenic distillation is carried out by mass and heat transfer between vapor and liquid phases that flow in countercurrent. The cryogenic distillation column comprises a boiler that produces the necessary amount of vapors along the column, plates or pack-age where the isotopic transfer between the vapors' and liquid take place and a condenser that provides the liquid reflux along the cryogenic distillation column. In the case of multi-component gas mixtures, determining the transport of the molecular species between the two phases is difficult due to the dependence of the physical-chemical properties of each mixture component. The transport of the molecular species is strongly influenced by the hydrodynamics of the two phases, closely connected with the size of the exchange interface

Study and analyses of practical plant performance through computer aided programs has better and cost effective. Aspen Hysys by Aspen Technology is one of the major process simulators that are widely used in cryogenic, chemical and thermodynamic process industries today. In this work, the simulation study of cryogenic air separation unit is performed by using Aspen Hysys. The simulation study is based on both steady state and dynamic (high pressure column and low pressure column)

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Chapter 1

Introduction

Cryogenic distillation is preferred to other methods of gas separation at industrial scale because it has the advantage of high separation factors, the possibility to process large amounts of gas while obtaining high purity gases. Similar with the conventional distillation processes, separation by cryogenic distillation is carried out by mass and heat transfer between vapor and liquid phases that flow in countercurrent. The cryogenic distillation column comprises a boiler that produces the necessary amount of vapors along the column, plates or pack-age where the isotopic transfer between the vapors' and liquid take place and a condenser that provides the liquid reflux along the cryogenic distillation column. In the case of multi-component gas mixtures, determining the transport of the molecular species between the two phases is difficult due to the dependence of the physical-chemical properties of each mixture component. The transport of the molecular species is strongly influenced by the hydrodynamics of the two phases, closely connected with the size of the exchange interface

The vapor liquid interface depends on the constructive characteristics of the separation medium: plates or package. In addition, in the case of hydrogen isotopes mixtures, the problem is complicated by the non-idealities in the thermodynamic properties near the saturation curve at low temperatures. A cryogenic distillation facility and is based on a traditional analysis model of the exchange process, but is applied to the low temperatures range which is specific to hydrogen and its isotopes.

1.1 Distillation

Distillation is a process that separates two or more components into an overhead distillate and bottoms. The bottoms product is almost exclusively liquid, while the distillate may be liquid or a vapor or both. The separation process requires three things. First, a second phase must be formed so that both liquid and vapor phases are present and can contact each other on each stage within a separation column. Secondly, the components have different volatilities so that they will partition between the two phases to different extent. Lastly, the two phases can be separated

by gravity or other mechanical means. Distillation differs from absorption and stripping in that the second phase is created by thermal means (Seader, 1998).

Separation of the isotopes of hydrogen has always been an important unit operation in the field of nuclear energy production. For use as the coolant and moderator in pressurized heavy water based reactors (PHWRs) employing natural uranium oxide as the fissile material, the separation and concentration of heavy water from natural sources of light water is a well-known and mature process technology, using unit operations like vacuum distillation and catalytic exchange. For the fusion energy field, gaseous hydrogen isotopes like deuterium and tritium are the postulated fuels. The pure form of each isotope can be separated and recovered in a cryogenic distillation column cascade. For fusion applications, the deuterium-tritium streams are the desired products. Hydrogen isotopes have normal boiling points ranging from 20 to 25 K so a cryogenic refrigeration system based on helium as the working fluid is an auxiliary requirement. Thus, cryogenic distillation of hydrogen isotopes is a very energy intensive process

.

1.2 Types of Distillation Column

There are many types of distillation column. Each type has its own characteristic and is designed to perform its efficiency

1.2.1 Tray Column

Tray Columns utilize a pressure and temperature differential to separate the products. For most tray columns, the weir holds a liquid level of each tray. Figure 10 shows how the tray works. Liquid enters from the down-comer of the tray above. The vapor must overcome this liquid head to move up the column. On the tray the vapor and liquid are contacted becomes bubble or froth where the mass transfer takes place and then above the tray they are separated where froth flows over the outlet weir and vapor with the light volatile compound is disengaged.

Tray column performs well in high liquid and vapor loading. Tray have higher pressure drop than packed, and It also have high resistance to corrosion. There are five major types of tray column.

1.2.1.1 Bubble Cap Tray

A bubble cap tray is perforated flat which has a riser (chimney) for each hole cover with a cap mounted. Usually equipped with slots to allow the passage of vapor then the vapor will contact with liquid forming bubble on the next tray. It is able to operate at low vapor and liquid rates (less than 2 gpm per foot of average of flow width).

1.2.1.2 Sieve Deck Tray

Sieve deck tray is perforated plate with holes punched into the plate usually has holes 3/16 in to 1 in diameter. Vapor comes out from the holes to give a multi orifice effect. The vapor velocity keeps the liquid from flowing down through the holes (weeping). The number and hole size are based on vapor flow up the tower. The liquid flow is transported down the tower by down-comers, a dam and overflow device on the side on the plate. Sieve deck tray has a minimum capacity approximately 70%.

1.2.1.3 Dual flow tray

Dual flow is a sieve tray without downcomer. It designed with enough open area on the tray deck to eliminate stagnation and promote back mixing. Vapor move up to the tray above through the hole while the liquid turn down in the same hole that result maldistribution and low efficiency.

1.2.1.4 Valve Tray

Valve Tray is using valve which is rise as vapor rate increase and then reduce as vapor rate falls, this stop the liquid from weeping. Valve can be round or rectangular, with or without caging structured. Valve disk rise as vapor rate increase. Valve tray has minimum capacity approximately 60%.

1.2.1.5 Baffle Tray

The down-comers require a disengaging area to separate the liquid from the vapor. This area requires a minimum distance that normally sets the tray spacing. The liquid is required to travel across the deck to the next down-comer. Baffle tray has three type's tray, there are Shed Decks, Side to Side Trays, Disk and Donuts Tray.

1.2.2 Packed Column

Packed column utilize packing to contact between the phases (liquid-vapor) on the surface. Packed column performs well at low pressure, low liquid and vapor loading that make packed column have the most efficient in these terms. At high flow parameters the capacity and efficiency can significantly reduce, also in heavy fouling applications and corrosive condition. Packed column has less pressure drop than tray column and it reduce foaming since generates thin films instead of fine droplets for mass and heat transfer. Packed column is divided by Random, Structured and Grid Packed Columns which is generate a mass transfer area by providing a large surface area over (50%) which the liquid can transfer heat and mass to the vapor.

1.2.2.1 Random Packed Column

Random packing is packing of specific geometrical shapes which are dumped into the tower and orient themselves randomly. Random packing has more risk than structured packing and less ability to handle maldistributed liquid.

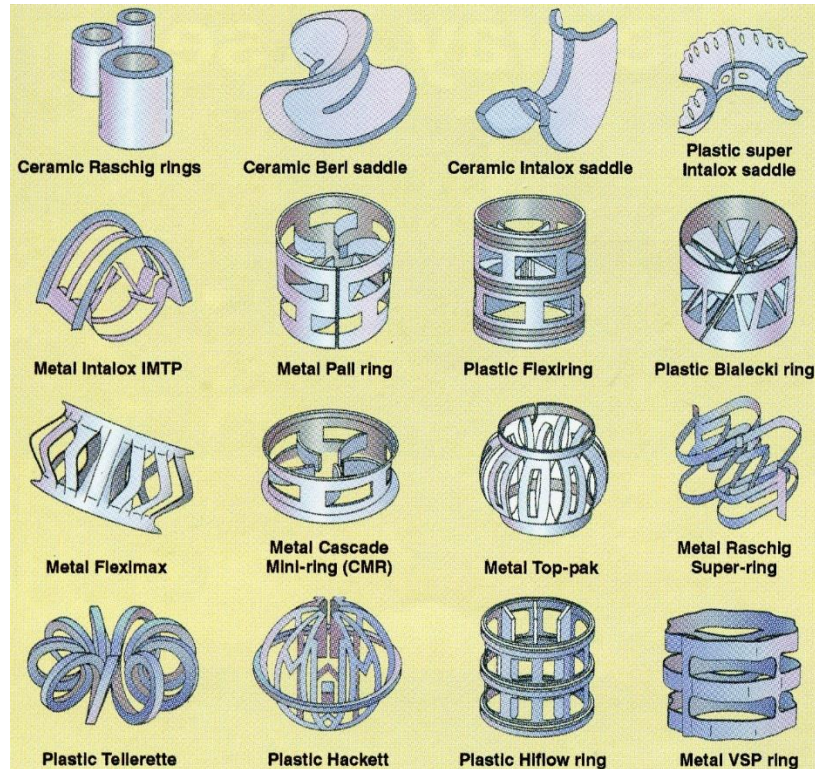


Figure 1.1: Types of random packing

1.2.2.2 Structured Packed Column

Structure Packed column is crimped layers or corrugated sheets which is stacked in the column. Each layer is oriented at 70° to 90° to the layer below. Structured packed offers 30% capacities higher than random packed for equal efficiency up to 50% higher at the same capacity.

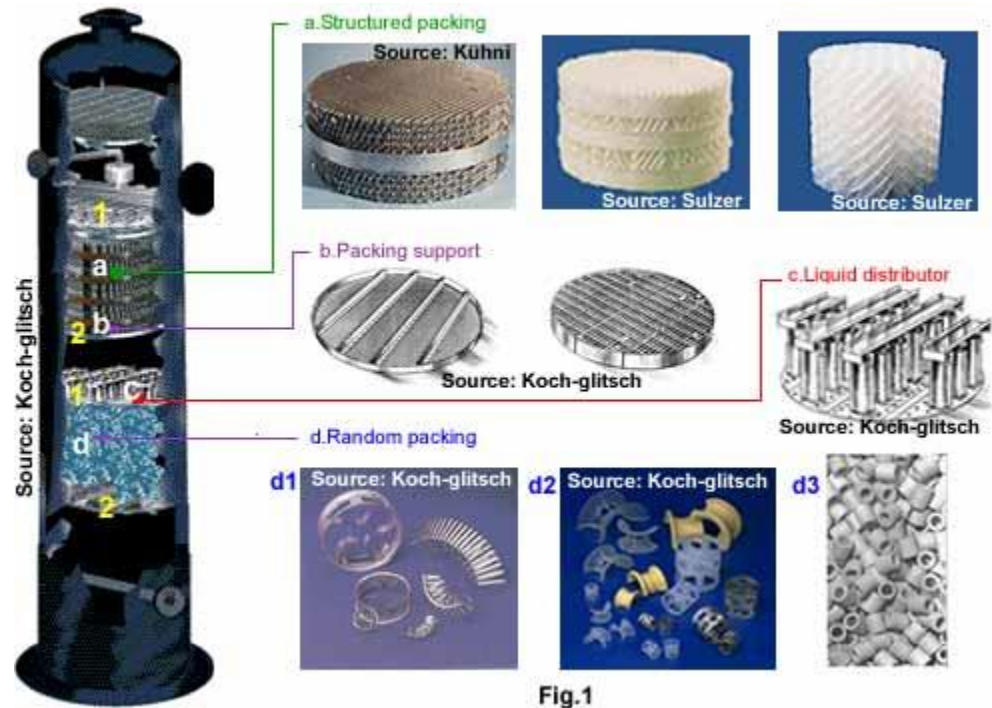


Figure 1.2: Types of structured packing

1.2.2.3 Grid Packed Column

Grid packed column is systematically arranged packing use an open-lattice structure. This device is composed of panels that promote mass transfer and enhance entrainment removal. They have high open area, resulting in high capacity, low pressure drop, and high tolerance to fouling

1.2.3 Packed Hydraulic

Packed tower operated under vapor-liquid counter current conditions and becoming increasingly important in environmental protection technologies. Among these, packing has received the

greatest attention owing to their good performance. That why the knowledge of the hydraulic characteristic are essential for design of packing tower to get the best optimizing performance of packing for maximizing theoretical stages per height of column, minimizing pressure drop per theoretical stage of separation, and maximizing the operating range of the column.

The operation area of packing is limited by the maximum loading which depend on the characteristic of phase, the type and geometry of the internal. Figure16 show the operating area of packed column.

The upper limit is called flooding point and the lower limit dewetting point. Reaching the loading point, the down flowing liquid phases holdback by the up flowing gas phase result a higher liquid in the bulk and increase the gas pressure drop then gives the flooding point. It make the liquid cannot flow downwards. While in the other side the vapor passes as single phase without contact to the liquid on the column. A strong segregation of the phases and a rapid increase of the pressure drop. Furthermore increase the loading and decrease of the efficiency

The area between loading point and flooding point is the operation area. The vapor can not pass the column without contact with liquid. Where the vapor is dispersed, some liquid is hold back. Because of high turbulence of both phases result a good mass transfer and high separation efficiency.

The lower limit is the minimum liquid flow or limit of wetting of the internals. With decreasing wetting of the internal, the mass transfer is reduced and separation efficiency of the column decreases. The lower limit is influenced by physical properties of the mixture to be separated as well as from material and geometry of the internals.

To control these limitations is used hydraulic mechanism. The study on hydraulic on packing included the pressure drop over the dry and wetted (irrigated) packing as well as dynamic (free draining) liquid hold up.

1.2.3.1 Pressure drop

The pressure drop is entirely by frictional losses through a series of opening and therefore is proportional to the square of the gas flow rate. In random packing, the opening are randomly sized and located, and pressure drop is due to expansion, contraction, and changes of direction. In structured packing, the openings are regular and uniform size and pressure drop is due to changes in direction. If a packed with gas flow is wetted on the surface of the internal liquid films are produced. The down flowing liquid reduced the relative voids volume, the free are for passing vapor is reduced and the vapor pressure drop is increases. Increasing wetting density will increase the liquid below loading zone which independent from vapor velocity.

1.2.3.2 Liquid holdup

The liquid holdup is the fraction of liquid held up in packed column. The volume of liquid holdup volume is often needed for calculating packed bed support beam loadings as well as for determining how much liquid drains to the bottom of a tower when the vapor rate is stopped.

1.2.3.3 Liquid rate

At lower liquid rates, irrigation to the bed is poor result poor efficiency. When liquid is well distributed in the column result the minimum wetting rate of the packing. Below minimum wetting the falling liquid film breaks up, some of the packing surface unwets, and the efficiency drops. When liquid distributor is poor, it will take more liquid to wet the entire packing bed.

1.2.3.4 Vapor rate

When vapor rate increases, column operation moves into the loading region. Efficiency improves because of the greater liquid holdup, but this improvement is short-lived. As the flood point is approached, the efficiency passes through the maximum and the drops because of excessive entrainment. When vapor rate decreases, it will decrease pressure drop per theoretical stage, but will increase column diameter.

1.2.4 General Design Consideration

A tower design is normally divided into two main steps, a process design followed by a mechanical design. The purpose of the process design is to calculate the number of required theoretical stages, column diameter and tower height. On the other hand, the mechanical design focuses on the tower internals and heat exchanger arrangements.

Many factors have to be considered in designing a distillation column such as the safety and environmental requirements, column performance, economics of the design and other parameters, which may constrain the work.

The first step in distillation column design is to determine the separation sequences, which depends on the relative volatility and concentration of each component in the feed. King has outlined a few design rules as follows:

- 1) Direct sequences that remove the components one by one in the distillate are generally favored.
- 2) Sequences that result in a more equal-molar division of the feed between distillate and bottoms products should be favored.
- 3) Separations where the relative volatility of two adjacent components is close to unity should be performed in the absence of other components; ie, reserve such a separation until the last column in the sequence.
- 4) Separations involving high-specified recovery fractions should be reserved until last in the sequence. Once the separation sequence is decided, engineering calculations follow to determine the number of theoretical stages, operating parameters and tower dimensions.

In general, the steps included in distillation calculations are summarized into the following:

- 1) Performing a material balance for the column
- 2) Determining the tower operating pressure (and/or temperature)
- 3) Calculating the minimum number of theoretical stages using the Fenske equation

- 4) Calculating the minimum reflux rate using the Underwood equations
- 5) Determining the operating reflux rate and number of theoretical stages
- 6) Selection of column internals (tray or packings)
- 7) Calculating the tower diameter and height

The theoretical explanation and sample calculations of each step above are discussed in detail in later sections.

Some general design rules that should be considered are as follows:

- 1) Distillation is usually the most economical method of separating liquids.
- 2) For Ideal mixtures (low pressure, medium temperature, and non-polar), relative volatility is the ratio of vapor pressures i.e. $\alpha = P_2/P_1$
- 3) Tower operating pressure is determined most often by the temperature of the available cooling medium in the condenser or by the maximum allowable reboiler temperature.
- 4) Tower Sequencing
 - A. Easiest separation first – least trays and reflux B.
 - B. When neither relative volatility nor feed concentrations vary widely, remove components one by one as overhead products..
 - C. When the adjacent ordered components in the feed vary widely in relative volatility, sequence the splits in order of decreasing volatility.
 - D. When the concentration in the feed varies widely but the relative volatilities do not, remove the components in the order of decreasing concentration in the feed.
- 5) Economically optimum reflux ratio is about 120% to 150% of the minimum reflux

- 6) The economically optimum number of stages is about 200% of the minimum value.
- 7) A safety factor of at least 10% above the number of stages by the best method is advisable.
- 8) A safety factor of at least 25% about the reflux should be utilized for the reflux pumps.
- 9) Reflux drums are almost always horizontally mounted and designed for a 5 min holdup at half of the drum's capacity.
- 10) For towers that are at least 3 ft (0.9 m) in diameter, 4 ft (1.2 m) should be added to the top for vapor release and 6 ft (1.8 m) should be added to the bottom to account for the liquid level and reboiler return.
- 11) Limit tower heights to 175 ft (53 m) due to wind load and foundation considerations.
- 12) The Length/Diameter ratio of a tower should be no more than 30 and preferably below 20.
- 13) A rough estimate of reboiler duty as a function of tower diameter is given by:

$$Q = 0.5 D^2 \text{ for pressure distillation}$$

$$Q = 0.3 D^2 \text{ for atmospheric distillation}$$

$$Q = 0.15 D^2 \text{ for vacuum distillation}$$

.

Where,

Q: Energy in Million Btu/hr

D: Tower diameter in feet.

The Selection of Column Internals

The selection of column internals has a big impact on the column performance and the maintenance cost of a distillation tower.

There are several choices of column internals and the two major categories are trays and packing. The choice of which to utilize depends on the

- 1) Pressure,
- 2) Fouling potential,
- 3) Liquid to vapor density ratio,
- 4) Liquid loading, and
- 5) Most importantly the life cycle cost.

Trays can be divided into many categories, such as baffle trays, dual flow trays, conventional trays, high capacity trays, multiple downcomer trays and system limit trays. According to some rules of thumb, trays should be selected if:

- 1) The compounds contain solids or foulants
- 2) There are many internal transitions
- 3) Liquid loads are high
- 4) There is a lack of experience in the service
- 5) Vessel wall needs periodic inspection
- 6) There are multiple liquid phases

On the other hand, packing divisions include grid packing, random packing, conventional structured packing, and high capacity structured packing. The rules of thumb for selecting packing are:

- 1) The compounds are temperature sensitive
- 2) Pressure drop is important (vacuum service)
- 3) Liquid loads are low
- 4) Towers are small in diameter
- 5) Highly corrosive service (use plastic or carbon)
- 6) The system is foaming
- 7) The ratio of tower diameter to random packing is greater than 10

Some design guidelines should be considered when designing a tray tower, such as follows:

- 1) Constriction factor the constriction factor should not be less than 0.6. This parameter shall be checked only for the side downcomer.
- 2) Tray spacing. Overall column heights depend on tray spacing. Tray spacing should be from 18 to 24 inches, with accessibility in mind (Generally, for a tower diameter of 4 feet and above, the most common tray spacing is 24 inches to allow easy access for maintenance. However, for a tower diameter below 4 feet, a tray spacing of 18 inches is adequate as the column wall can be reached from the midway.)
- 3) Peak tray efficiencies usually occur at linear vapor velocities of 2 ft./s (0.6 m/s) at moderate pressures, or 6 ft./s (1.8 m/s) under vacuum conditions.
- 4) A typical pressure drop per tray is 0.1 psi (0.007 bars). Max Dry pressure drop in height of hot liquid less than 16% of tray spacing.
- 5) Tray efficiencies for aqueous solutions are usually in the range of 60-90% while gas absorption and stripping typically have efficiencies closer to 10-20%
- 6) Sieve tray holes The generally vary are 0.25 to 0.50 in. diameter with the total hole area being about 10% of the total active tray area. Maximum efficiency is 0.5 in and 8%. Those large holes are recommended for fouling and corrosive services and a spray regime.
- 7) Valve trays Valve tray typically has 1.5 in and 2 in. diameter holes each with a lifting cap. 12- 14 caps/square foot of tray is a good benchmark. The disk typically rises 3/16 to 7/16 in above the tray deck and 10 % open area of fully open valves.
- 8) Weir height the most common weir heights are 2 to 3 in and the weir length is typically 75% of the tray diameter. For vacuum operation is recommended 0.25 to 0.5 in to reduce the pressure drop.
- 9) Weir loading the maximum recommended weir loading is 13 gpm/inch. At high weir loadings, trays will have high pressure drop, high froth height and potential downcomer limitations. At lower weir loading, picket fencing may be required.

10) Downcomer clearance it is recommended 1.5 in. At low liquid loading the clearance can be reduced to secure a proper distribution of the liquid on the active area, but lower than 1 in are not recommended. At high liquid loading the clearance can be increased up to the weir height to minimize the head loss and the jetting.

11) Downcomer velocity and residence time the velocity is range from 0.1-0.7 ft./s, the maximum velocity needs to be low enough to prevent downcomer flooding. The minimum residence time is 3 s and the best residence time is 5 s. the residence time needs to be long enough to allow adequate vapor-liquid disengagement.

12) Flow path length the flow path length is measured from the downcomer exit to the outlet weir. Minimum size is typically 16 to 18 inches. High flow path length will enhance the efficiency while the low flow path length will increase weir load.

13) Open area Open area typically 0.04 to 0.15. lower values may result hydraulic limitation and mass transfer efficiency reduced while higher value result less the tray efficiency.

The packed tower design concepts are listed below:

- 1) Packed towers almost always have lower pressure drop compared to tray towers.
- 2) Packing is often retrofitted into existing tray towers to increase capacity or separation.
- 3) For gas flow rates of 500 ft³ /min (14.2 m³ /min), use 1 in (2.5 cm) packing, for gas flows of 2000 ft³ /min (56.6 m³ /min) or more, use 2 in (5 cm) packing.
- 4) Ratio of tower diameter to packing diameter should usually be at least 15
- 5) Due to the possibility of deformation, plastic packing should be limited to an unsupported depth of 10-15 ft (3-4 m) while metal packing can withstand 20-25 ft (6-7.6 m).
- 6) Liquid distributor should be placed every 5-10 tower diameters (along the length) for pall rings and every 20 ft (6.5 m) for other types of random packing.

- 7) For redistribution, there should be 8-12 streams per sq. foot of tower area for towers larger than three feet in diameter. They should be even more numerous in smaller towers.
- 8) Packed columns should operate near 70% flooding.
- 9) Height Equivalent to Theoretical Stage (HETS) for vapor-liquid contacting is 1.3- 1.8 ft (0.4- 0.56 m) for 1 in pall rings and 2.5-3.0 ft (0.76-0.90 m) for 2 in pall rings.
- 10) Design pressure drops should be as follows:

Table 1.1: Service vs Pressure drop (in water/ft. packing)

Service	Pressure Drop (in water/ft. packing)
Absorbers and Regenerators	
Non-Foaming Systems	0.25 - 0.40
Moderate Foaming Systems	0.15 - 0.25
Fume Scrubbers	
Water Absorbent	0.40 - 0.60
Chemical Absorbent	0.25 - 0.40
Atmospheric or Pressure Distillation	0.40 - 0.80
Vacuum Distillation	0.15 - 0.40
Maximum for Any System	1.0

- 11) Packing support is used to carry the weight of the wet packing while allowing free passage of the gas and liquid. Gas inlets are provided above the level where the liquid flows from the bed.

12) Liquid distributor is used to maintaining a uniform flow of liquid throughout the column. For small diameter columns, a central open feed pipe or one fitted with a spray nozzle may well be adequate.

13) Liquid redistributors Redistributors are used to collect liquid that has migrated to the column walls and redistribute it evenly over the packing and out any misdistribution.

Chapter 2

Literature review

Introduction

A literature survey helps in summarizing the current knowledge in the area of investigation, identifying any strengths and weaknesses in previous work, which in turn helps you to identify them in your own research and thus serving to you to spot them in your own analysis and so eliminate the potential weaknesses, whilst bringing to the fore the potential strengths. Additionally, a decent and full literature search can offer the context within which to place your study.

1. Mass Transfer in Cryogenic Distillation Column Separating Hydrogen Isotopes

A simulation model was proposed to study the mass and heat transfer rates in hydrogen isotope distillation columns. The model is on the basis of the analogy: the mass transfer coefficients and effective surface area within the column were estimated by Kosuge's and Onda's correlation in the model. The calculated results by the present model agreed approximately with the experimental observations. The model had a tendency to give slightly higher separation performance. This tendency is due to that the estimated effective surface area might be larger than actual values. The calculated results by the proposed model were compared with those by the stage model also to discuss relationship between the mass transfer rate and the HETP value. The estimated mass transfer rates were almost the same for H-D and D-T systems. This calculated result give a reason why the HETP values were not varied for the difference in physical properties of hydrogen isotopes. The proposed model does not have the parameter that fit the calculated results to the experimental observations. Comparing the calculated results by the proposed model with those by the stage model, we can estimate the HETP value.

1. Simulation studies of the characteristics of a cryogenic distillation column for hydrogen isotope separation

Cryogenic distillation is a very widely applied technique for separating the components of a mixture of hydrogen isotopes, which may contain up to six isotopic species. This work presents a simple dynamic model for evaluating the major performance characteristics of a cryogenic distillation column for hydrogen isotope separation. Liquid hold up, pressure drop and flooding point have been predicted for the tower using known packing characteristics and fluid properties. The column has been modelled as an equivalent tray tower using a known value of the height equivalent to theoretical plate (HETP) and its dynamic behaviour and separation performance under various conditions have been predicted. The effect of parameters like temperature, reflux ratio, feed point location and feed composition on the final isotopic contents of top and bottom products at steady state has also been studied. Consequences of neglecting the decay heat of tritium in distillation calculations have also been evaluated. This model is intended for preliminary column design work using data from literature, without the need for prior experimental activity.

2. H-D-T cryogenic distillation experiments at TPL/JAERI in support of ITER

The hydrogen isotope separation system (ISS) using cryogenic distillation method is one of the key systems in a fuel cycle loop of a fusion reactor. The ISS for the International Thermonuclear Experimental Reactor (ITER), is characterized by its required flexibility for the variability of feed composition, which is not considered in the existing industrial distillation columns, so that the development of evaluation method of dynamic behavior, which is the base for the establishment of ISS control system, is essential as original technology. At the Tritium Process Laboratory in Japan Atomic Energy Research Institute (TPL/JAERI), H-D-T cryogenic distillation experiments have been carried out to acquire the systematic data for the design of the ISS for the ITER. The value of height equivalent to a theoretical plate [Y. Iwai, T. Yamanishi, S. O'hira, T. Suzuki, W.M. Shu, M. Nishi,2002]

(HETP) was estimated to be 5 cm by the results of present experiments and it was adopted in the ITER_ ISS design. The in situ, multi-points and reliable high-speed gas analytical system with Laser Raman spectroscopy was successfully demonstrated in the experiment to analyze the experiment.

Chapter 3

Introduction to ASPEN Hysys

HYSYS is a powerful engineering simulation tool, has been uniquely created with respect to the program architecture, interface design, engineering capabilities, and interactive operation. The integrated steady state and dynamic modeling capabilities, where the same model can be evaluated from either perspective with full sharing of process information, represent a significant advancement in the engineering software industry.

The various components that comprise HYSYS provide an extremely powerful approach to steady state modeling. At a fundamental level, the comprehensive selection of operations and property methods allows you to model a wide range of processes with confidence. Perhaps even more important is how the HYSYS approach to modeling maximizes your return on simulation time through increased process understanding.

To comprehend why HYSYS is such a powerful engineering simulation tool, you need look no further than its strong thermodynamic foundation. The inherent flexibility contributed through its design, combined with the unparalleled accuracy and robustness provided by its property package calculations leads to the presentation of a more realistic model.

HYSYS is widely used in universities and colleges in introductory and advanced courses especially in chemical engineering. In industry the software is used in research, development, modeling and design. HYSYS serves as the engineering platform for modeling processes from Upstream, through Gas Processing and Cryogenic facilities, to Refining and Chemicals processes.

There are several key aspects of HYSYS which have been designed specifically to maximize the engineer's efficiency in using simulation technology. Usability and efficiency are two obvious attributes, which HYSYS has and continues to excel at. The single model concept is key not only to the individual engineer's efficiency, but to the

efficiency of an organization.

Books about HYSYS are sometimes difficult to find. HYSYS has been used for research and development in universities and colleges for many years. In the last few years, however, HYSYS is being introduced to universities and colleges students as the first (and sometimes the only) computer simulator they learn. For these students there is a need for a book that teaches HYSYS assuming no prior experience in computer simulation.

Aspen Plus, Aspen HYSYS, ChemCad and MATLAB, PRO/II™ etc. are the commonly used process simulators for modeling, simulation and optimization of a distillation process in the chemical industries.^{[1][2]} Distillation is the technique of preferential separation of the more volatile component (s) from the less volatile ones in a feed followed by condensation. The vapor produced is richer in the more volatile components(s). The distribution of the component in the two phase is governed by the vapour-liquid equilibrium relationship. In practice, distillation may be carried out by either two principal methods. The first method is based on the production of vapor boiling the liquid mixture to be separated and condensing the vapors without allowing any liquid to return to the still. There is no reflux. The second method is based on the return of part of the condensate to still under such conditions that this returning liquid is brought into intimate contact with the vapors on their way to condenser.

A simulation is the representation of the real world process or system over a period of time. Simulation can be done by hand or on a computer, simulation involves the generation of artificial history of the system and the observation of artificial history to draw inferences concerning of the operating characteristic of the real system. Thus, simulation modelling can be used both as an analysis tool for predicating the effect of changes to existing system and as a design tool to predict the performance of new system under the varying set of circumstances.^[7] Process simulation describes processes flow diagram where various unit operations are present and connected by product streams.

It is extensively used both in educational arena and industry to predicate the behavior of a process using material balance equations, equilibrium relationship, reaction kinetics, etc.

Chapter 4

Designing of the Column

4.1 Mc-Cabe Thiele Method

McCabe and Thiele (1925) developed a graphical method to determine the theoretical number of stages required to affect the separation of a binary mixture (McCabe and Smith, 1976). This method uses the equilibrium curve diagram to determine the number of theoretical stages (trays) required to achieve a desired degree of separation. It assumes constant molar overflow and this implies that: (i) molal heats of vaporization of the components are roughly the same; (ii) heat effects are negligible. The information required for the systematic calculation are the VLE data, feed condition (temperature, composition), distillate and bottom compositions; and the reflux ratio, which is defined as the ratio of reflux liquid over the distillate product. For example, a column is to be designed for the separation of a binary mixture as shown in Figure

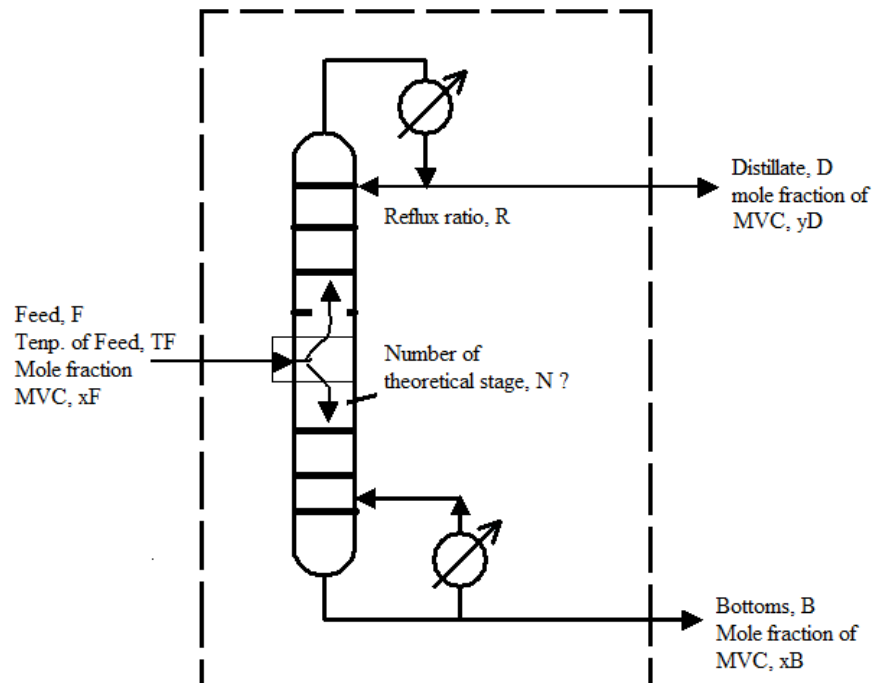


Figure 4.1: Schematic of column for separation of binary mixture

The feed has a concentration of x_F (mole fraction) of the more volatile component, and a distillate having a concentration of x_D of the more volatile component and a bottoms having a concentration of x_B is desired. In its essence, the method involves the plotting on the equilibrium diagram three straight lines: the rectifying section operating line (ROL), the feed line (also known as the q-line) and the stripping section operating line (SOL). An important parameter in the analysis of continuous distillation is the Reflux Ratio, defined as the quantity of liquid returned to the distillation column over the quantity of liquid withdrawn as product from the column, i.e. $R = L / D$. The reflux ratio R is important because the concentration of the more volatile component in the distillate (in mole fraction x_D) can be changed by changing the value of R . The steps to be followed to determine the number of theoretical stages by McCabe-Thiele Method:

- Determination of the Rectifying section operating line (ROL).
- Determination the feed condition (q).
- Determination of the feed section operating line (q -line).
- Determination of required reflux ratio (R).
- Determination of the stripping section operating line (SOL).
- Determination of number of theoretical stage.

Determination of the Rectifying section operating line (ROL)

Overall balance:

$$V_{n+1} = L_n + D \tag{1}$$

Component Balance for more volatile component:

$$V_{n-1}y_{n-1} = L_nx_n + Dx_D \tag{2}$$

$$(L_n + D)y_{n+1} = L_nx_n + Dx_n \tag{3}$$

Consider the constant molal flow in the column, and then one can write: $L_1=L_2= \dots$
 $\dots L_{n-1} = L_n = L_{n+1} = L = \text{constant}$ and $V_1= V_2= \dots V_{n-1}= V_n= V_{n+1}=V=\text{constant}$.

Thus, the equation(3) becomes:

$$(L+D)y_{n+1} = Lx_n + Dx_D \tag{4}$$

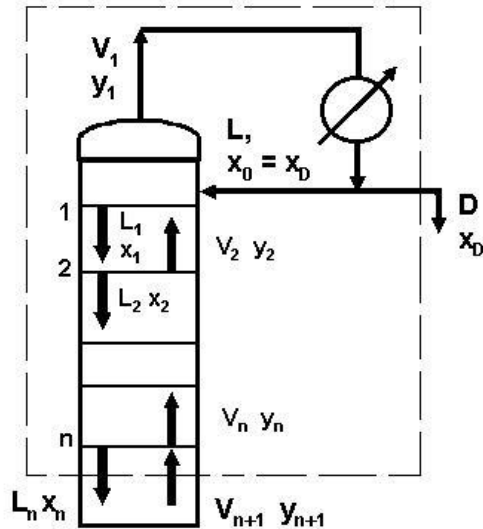


Figure 4.2: Outline graph of rectifying section

After rearranging, one gets from the equation (4):

$$Y_{n+1} = \left(\frac{L}{L+D}\right) x_n + \left(\frac{D}{L+D}\right) x_D \tag{5}$$

Introducing reflux ratio defined as: $R = L/D$, the Equation (5) can be expressed as:

$$Y_{n+1} = \left(\frac{R}{R+1}\right) x_n + \left(\frac{1}{R+1}\right) x_D \tag{6}$$

The Equation is the rectifying section operating line (ROL) Equation having slope $R/(R+1)$ and intercept, $x_D/(R+1)$ as shown in Figure 4. If $x_n = x_D$, then $y_{n+1} = x_D$, the operating line passed through the point (x_D, x_D) on the 45° diagonal line. When the reflux ratio R changed, the ROL will change. Generally, the rectifying operating line is expressed without subscript of n or $n+1$. Without subscript the ROL is expresses as:

$$Y = \left(\frac{R}{R+1}\right)x + \left(\frac{1}{R+1}\right)x_D \quad (7)$$

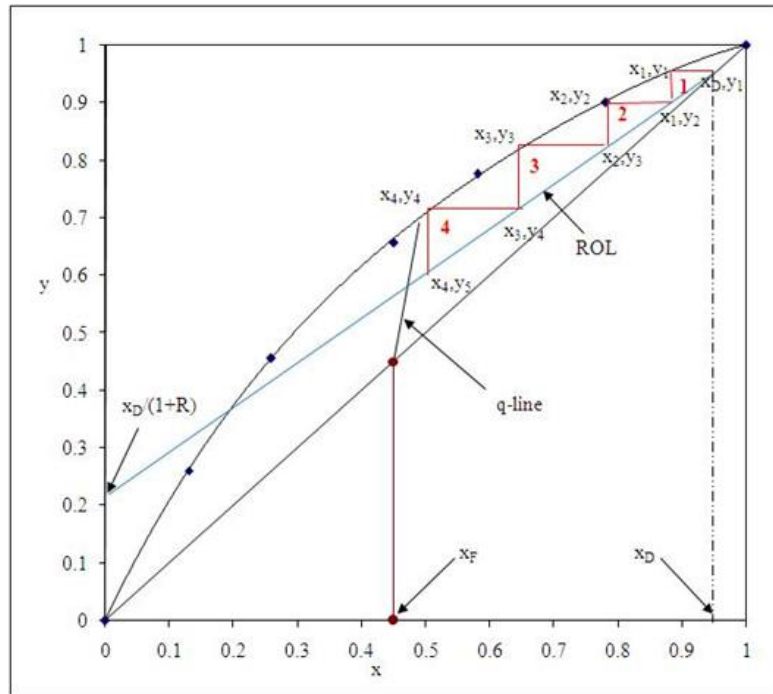


Figure 4.3: Representation of the rectifying operating line

Determination the feed condition (q):

The feed enters the distillation column may consists of liquid, vapor or a mixture of both. Some portions of the feed go as the liquid and vapor stream to the rectifying and stripping sections. The moles of liquid flow in the stripping section that result from the introduction of each mole of feed, denoted as 'q'. The limitations of the q-value as per feed conditions are shown in Table 1.

Table 4.1: Limitations of q-value as per feed conditions

Feed condition	Limit of q-value
cold feed (below bubble point)	$q > 1$
feed at bubble point (saturated liquid)	$q = 1$
feed as partially vaporized	$0 < q < 1$
feed at dew point (saturated vapor)	$q = 0$
feed as superheated vapor	$q < 0$
feed is a mixture of liquid and vapor	q is the fraction of the feed that is liquid

Calculation of q-value

When feed is partially vaporized:

Other than saturated liquid ($q = 1$) and saturated vapor ($q = 0$), the feed condition is uncertain. In that case one must calculate the value of q. The q-value can be obtained from enthalpy balance around the feed plate. By enthalpy balance one can obtain the q-value from the following form of Equation:

$$q = \frac{H_v - H_F}{H_v - H_L} \quad (8)$$

Where H_F , H_v and H_L are enthalpies of feed, vapor and liquid respectively which can be obtained from enthalpy-concentration diagram for the mixture [Cristescu I, Ioana Cristescu, Poenariu V, Preda I, Stefan L, 2000].

When feed is cold liquid or superheated vapor:

q can be alternatively defined as the heat required to convert 1 mole of feed from its entering condition to a saturated vapor; divided by the molal latent heat of vaporization. Based on this definition, one can calculate the q-value from the following Equations for the case whereby $q > 1$ (cold liquid feed) and $q < 0$ (superheated vapor feed) as:

For cold liquid feed:

$$Q = \frac{c_{p,L}(T_{bP} - T_F) + \lambda}{\lambda} \quad (9)$$

For superheated vapor feed:

$$Q = \frac{c_{p,V}(T_{dP} - T_F)}{\lambda} \quad (10)$$

where T_{bp} is the bubble point, λ is the latent heat of vaporization and T_{dp} is the dew point of the feed respectively

Determination of the feed section operating line (q-line):

Consider the section of the distillation column (as shown in Figure 1) at the tray (called feed tray) where the feed is introduced. In the feed tray the feed is introduced at F moles/hr with liquid of q fraction of feed and vapor of (1-f) fraction of feed as shown in Figure. Overall material balance around the feed tray:

(11)

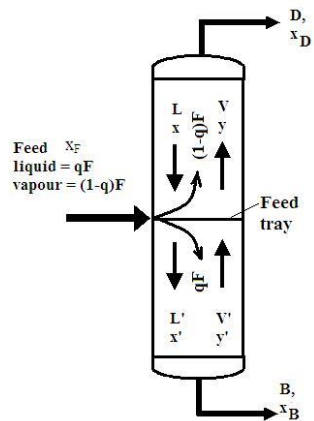


Figure 4.4: Feed tray with fraction of liquid and vapor of feed

From component balance around the entire column, it can be written as

$$Vy = Lx + Dx_D \quad (14)$$

Substituting $L-L'$ and $V-V'$ from Equations (12) and (13) into Equation (14) and with Equation (5.27) one can get the q -line Equation after rearranging as:

For a given feed condition, x_F and q are fixed, therefore the q -line is a straight line with slope $-q / (1-q)$ and intercept $x_F / (1-q)$. If $x = x_F$, then from Equation (5.28) $y = x_F$. At this condition the q -line passes through the point (x_F, x_F) on the 45° diagonal. Different values of q will result in different slope of the q -line. Different q -lines for different feed conditions are shown in Figure 5.15.

(15) $y = x_F$. At this condition the q -line passes through the point (x_F, x_F) on the 45° diagonal. Different values of q will result in different slope of the q -line. Different q -lines for different feed conditions are shown in Figure 5

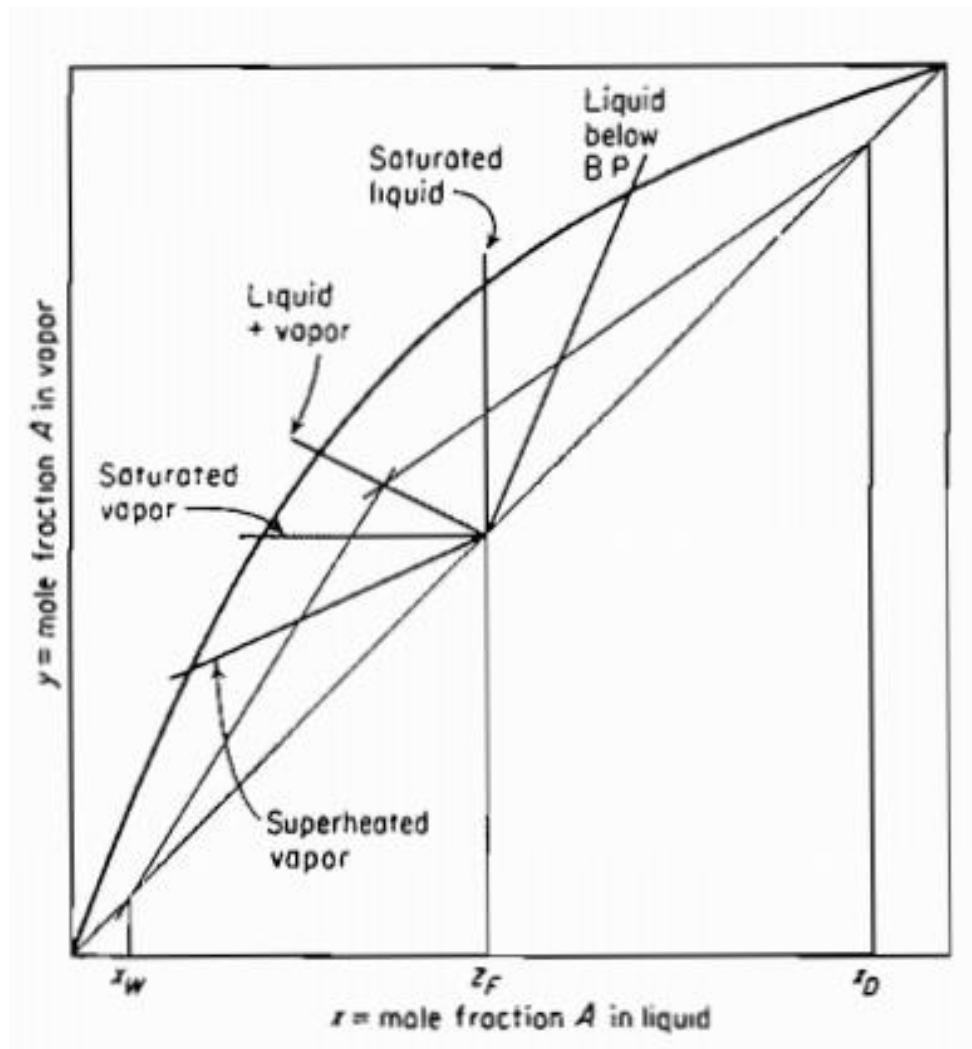


Figure 4.5: Different q-lines for different feed conditions

Calculation of the minimum reflux ratio

$$q=1 \quad R_m = \frac{1}{\alpha-1} \left[\frac{x_D}{x_F} + \alpha \frac{1-x_D}{1-x_F} \right]$$

$$q=0 \quad R_m = \frac{1}{\alpha-1}$$

4.2. Determination of the column height

4.2.1. The theoretical stage method

If at a point of the distillation column the concentration of the liquid flow is x , and the concentration of the counter-current vapor flow at the same point is y , then there is a height above this point where the concentration of the vapor flow (y^*) is in equilibrium with x . This section is the Height Equivalent a Theoretical Plate (*HETP*).

The height of the packing is calculated by Eq. 1.

$$H = HETP \cdot n \quad (1)$$

where n , number of theoretical stages (determined by the McCabe-Thiele method)

HETP Height Equivalent a Theoretical Plate [m]

H Height of the packing [m]

The value of the *HETP* can be determined by the modified Granville1 equation (Eq. 2).

$$HETP = 28 \cdot d_p \cdot m_a \cdot \frac{V}{L} \left(\frac{H}{2.4} \right)^{1/3} \quad (2)$$

Where, d_p diameter of the packing [m]
 m_a average slope of the equilibrium curve
 V molar vapor flow rate [kmol/h]
 L molar liquid flow rate [kmol/h]

The value of m_a can be determined by the following method:

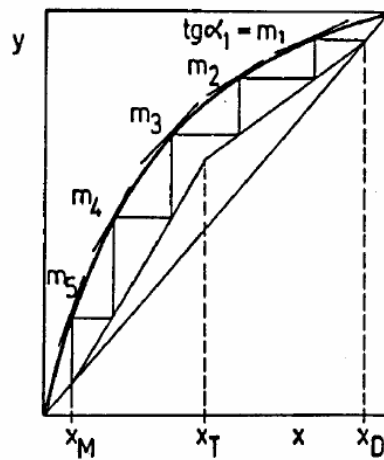


Figure 4.6 : The calculation of m_a

$$m_a = \frac{\sum_{i=1}^n m_i}{n} \quad (3)$$

Where, m_i local slope of the equilibrium curve at theoretical plate i .

4.2.2. The transfer unit method

The transfer unit is a part of column height where the change in vapor concentration equals to the average driving force. The driving force is the difference between the equilibrium (y^*) and the actual (y) vapor concentration.

The column height can be computed by Eq. 4.

$$H = HTU \cdot NTU \quad (4)$$

where HTU Height of a Transfer Unit [m]

NTU Number of Transfer Units

NTU can be determined by Eq. 5.

$$NTU = \int_{y_B}^{y_D} \frac{dy}{y^* - y} \quad (5)$$

where y_D vapor concentration at the top of the column

y_B vapor concentration at the bottom of the column

The relation between the equilibrium concentrations (y^*) and the actual concentrations (y) is shown in Figure 2. NTU can be determined by graphical integration, as it can be seen in Figure 3.

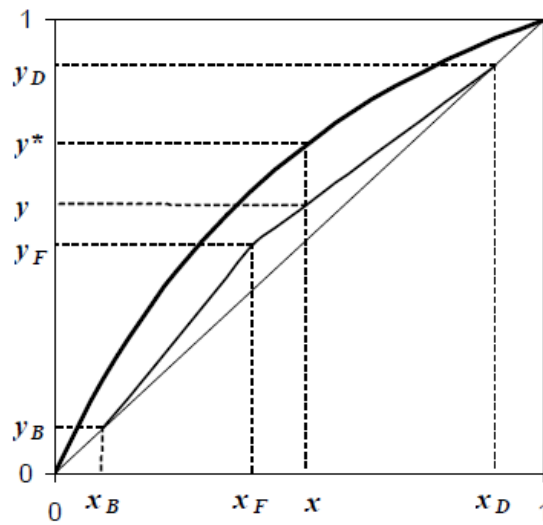


Figure 4.7. Relation between y^* and y

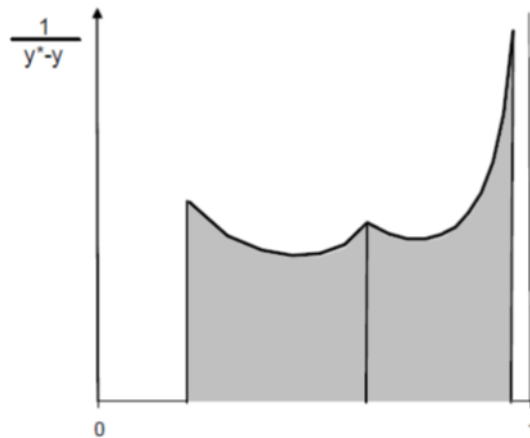


Figure 4.8. Graphical integration

There is no entirely satisfactory method for predicting the height of a transfer unit. In practice the value for a particular packing will depend not only on the physical properties and flow rates of the vapor and liquid, but also on the uniformity of the liquid distribution throughout the column, which depends on the height and diameter of the column.

Kasatkin published useful correlations for the mass-transfer coefficients K_V which can be used to calculate H . First, the equivalent diameter of the packing (d_e) must be calculated:

$$d_e = 4 \frac{\varepsilon}{\Omega} \quad (6)$$

where ε fractional voidage [m³ free volume / m³ column volume]
 Ω interfacial surface per unit volume of column [m²/m³]

After then the Archimedes (Ar) and the Reynolds (Re) numbers can be determined:

$$Ar = \frac{de^3(\rho_L - \rho_v)\rho_v g}{\eta_v^2} \quad (7)$$

$$Re = 0.15 Ar^{0.57} \left(\frac{V}{L}\right)^{0.43} \quad (8)$$

where ρ_L liquid density [kg/m³]
 ρ_v vapor density [kg/m³]
 η_v dynamic viscosity of vapor [Pa s]

The linear vapor velocity (v , [m/s]) can be calculated:

$$v = \frac{Re \eta_v}{d_e \rho_v} \quad (9)$$

After that the mass transfer coefficient (K_v , [1/s]):

$$k_v = 0.35Re^{0.8} \left(\frac{\eta_v}{\rho_v D_v} \right)^{0.35} D_v / d_e^2 \quad (10)$$

where D_v diffusivity of vapor [m/s]

The Height of the Transfer Unit is given by:

$$HTU = \frac{v}{k_v} \quad (11)$$

Chapter 5

Calculations

5.1 Graphical Method

Using Mc-Cabe thiele method to determine the number of stages for various feed conditions. There are different types of feed conditions. $q=1$ is Saturated liquid, $q=0$ is Saturated vapor, $Q<0$ Superheated Vapor, $q >1$ is liquid below BP and $1<q<0$ is liquid and vapor.

Table 5.1: Initial design Basis

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(gmole/day)	300

a. When $q = 1$

Table 5.2: X and Y data when $q=1$

X	Y
0	0
0.1	0.2659
0.2	0.449
0.3	0.5828
0.4	0.6848
0.5	0.7652
0.6	0.8302
0.7	0.8302
0.8	0.9287
0.9	0.967
1	1

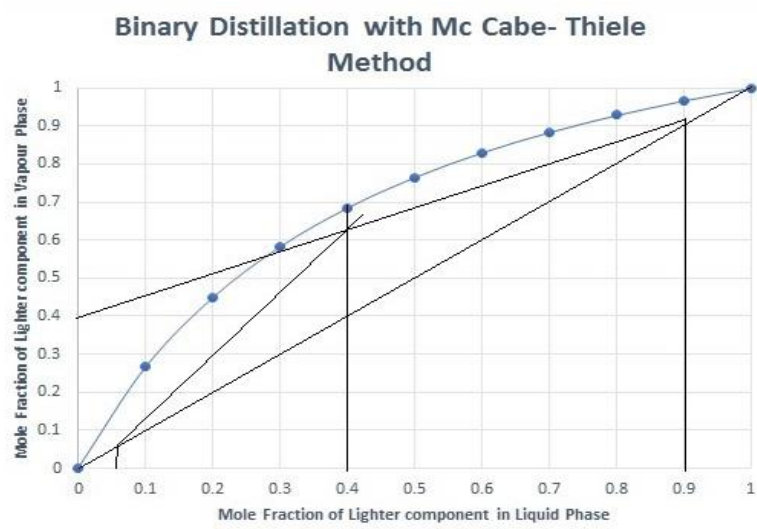


Figure 5.1: Mc Cabe – Thiele method for Saturated Liquid

b. When $q=0$,

Table 5.3: X and Y data when $q=0$

X	Y
0	0
0.1	0.22
0.2	0.38
0.3	0.52
0.4	0.62
0.5	0.71
0.6	0.79
0.7	0.856
0.8	0.91
0.9	0.95
1	1

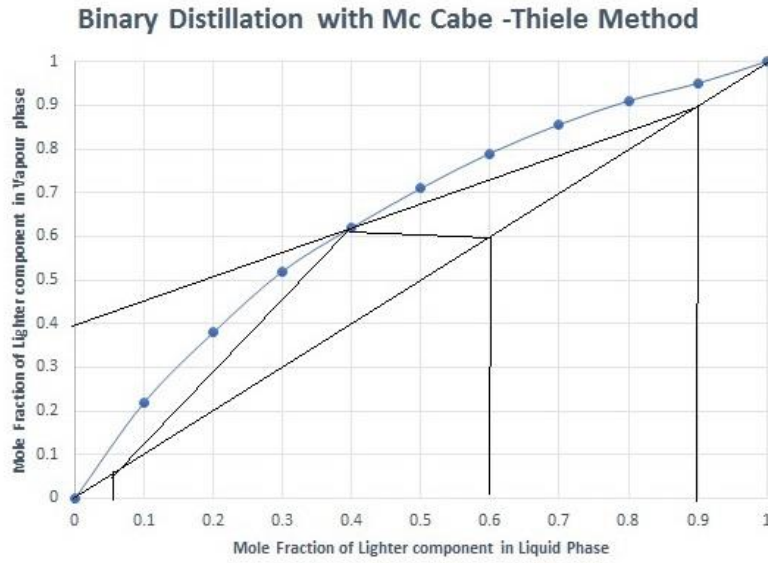


Figure 5.2: Binary Distillation with McCabe Thiele for Saturated vapor

c. When $0 < q < 1$

Table 5.4: X and Y data when $0 < q < 1$

X	Y
0	0
0.1	0.2429
0.2	0.4145
0.3	0.5514
0.4	0.6524
0.5	0.7376
0.6	0.8101
0.7	0.8709
0.8	0.92
0.9	0.9585
1	1

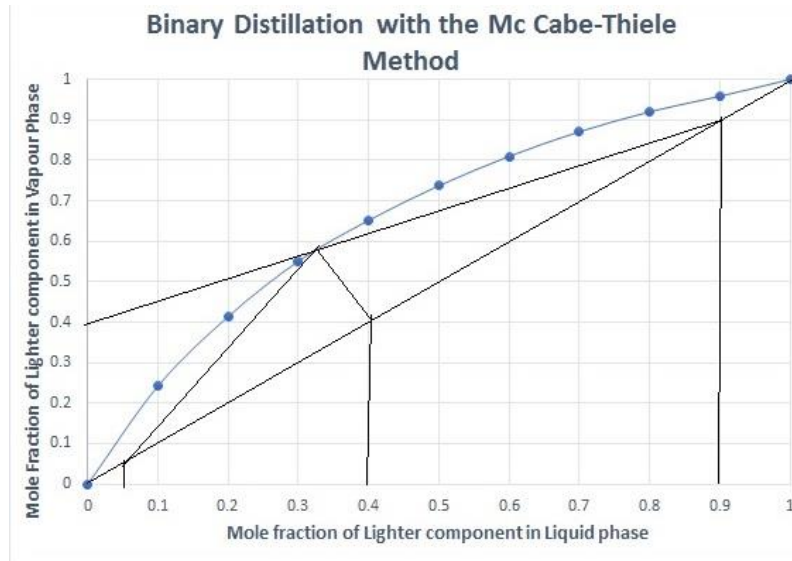


Figure 5.3: Binary Distillation with Mc Cabe-Thiele Method for partially liquid and vapor

Table 5.5: Determining the number of trays

Q-Line	Number of Trays
$Q=0$	13
$0 < Q < 1$	15
$Q=1$	7

5.2 Simulation Method

5.2.1 For Saturated liquid ($q=1$, 15K)

1. Feed(300gmole/day)

Table 5.6 : Initial Data basis for 300gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.0125
Reflux ratio	1.5
Number of Trays	10
Efficiency	60%

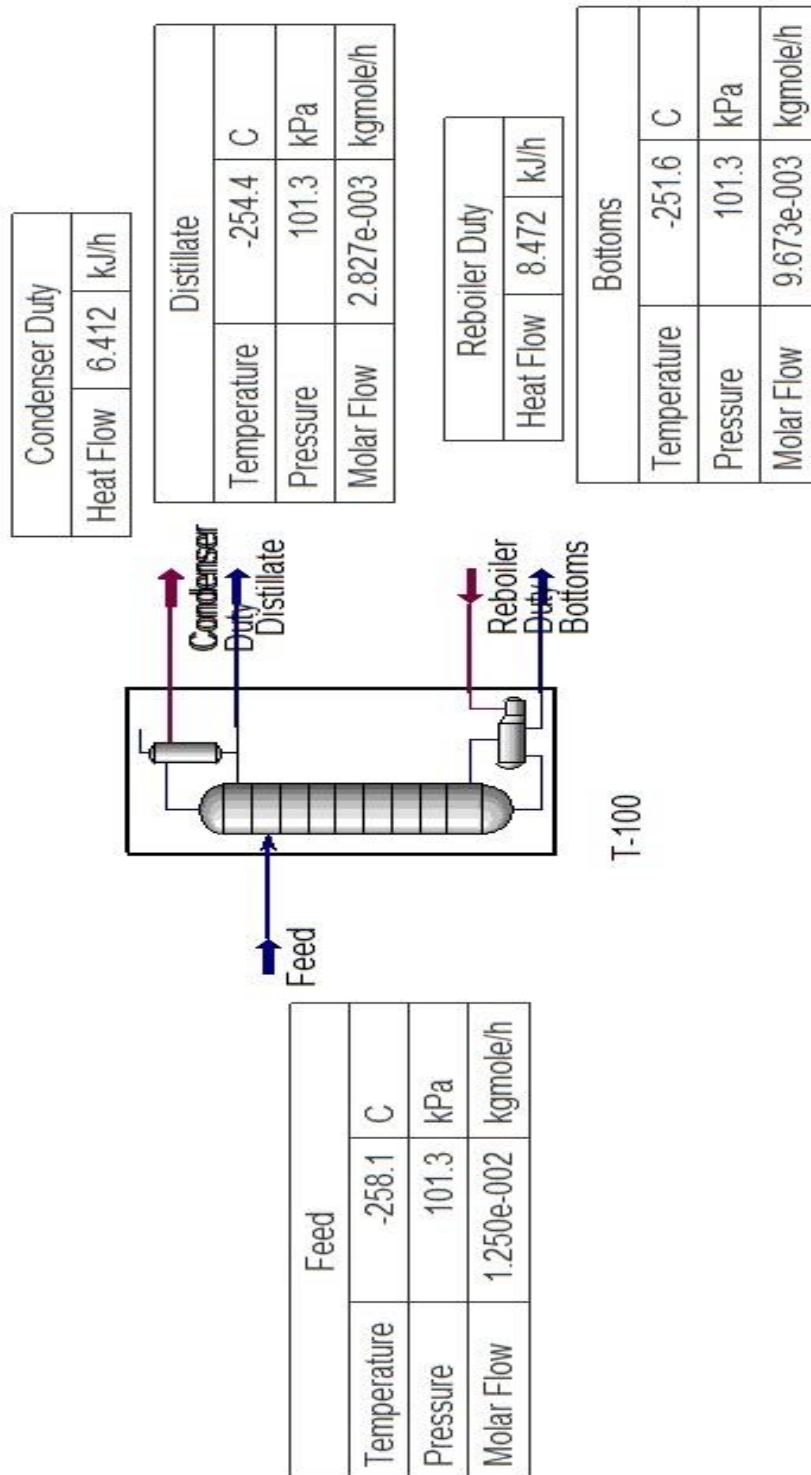


Figure 5.4: Flowsheet of the packed distillation column(15K,300gmole/day)

2. Feed (350gmole/day)

Table 5.7: Initial Data basis for 350gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.01458
Reflux ratio	1.5
Number of Trays	10
Efficiency	60%

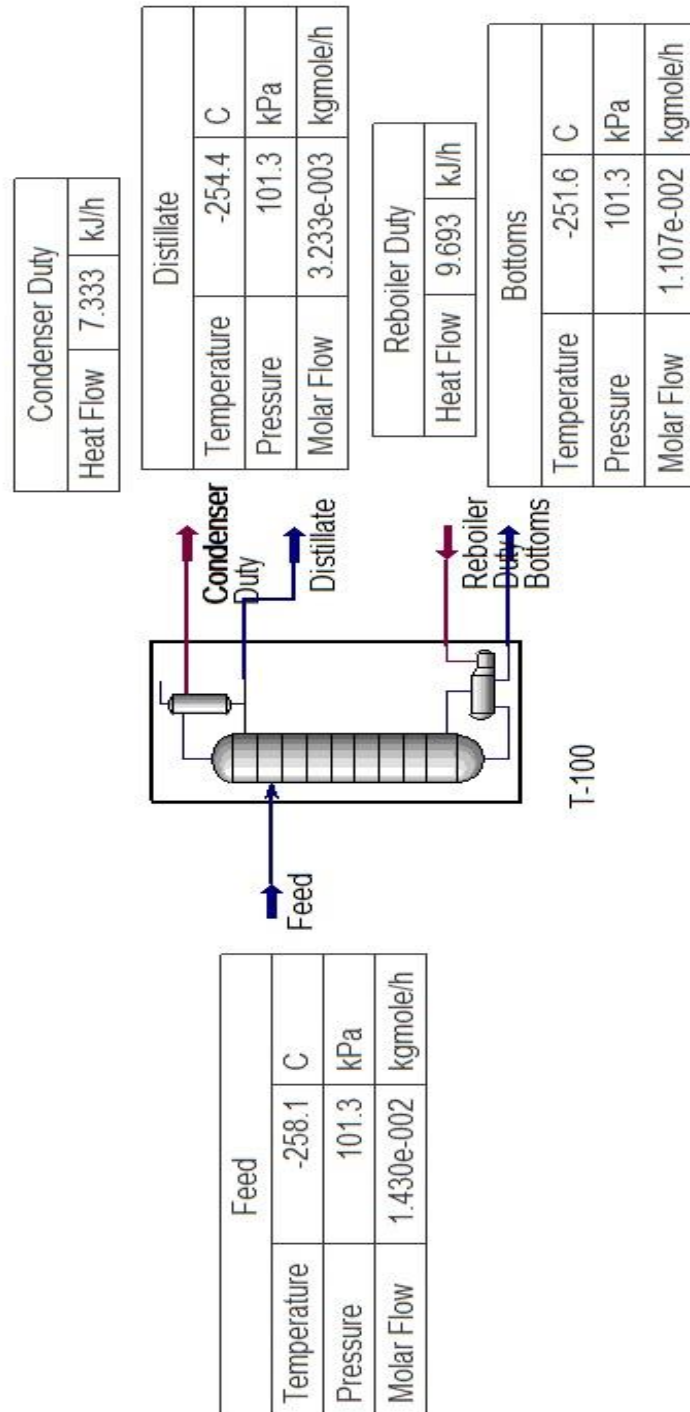


Figure 5.5: Flowsheet of the packed distillation column(15K,350gmole/day)

3. Feed (400gmole/day)

Table 5.8: Initial Data basis for 400gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.1666
Reflux ratio	1.5
Number of Trays	10
Efficiency	60%

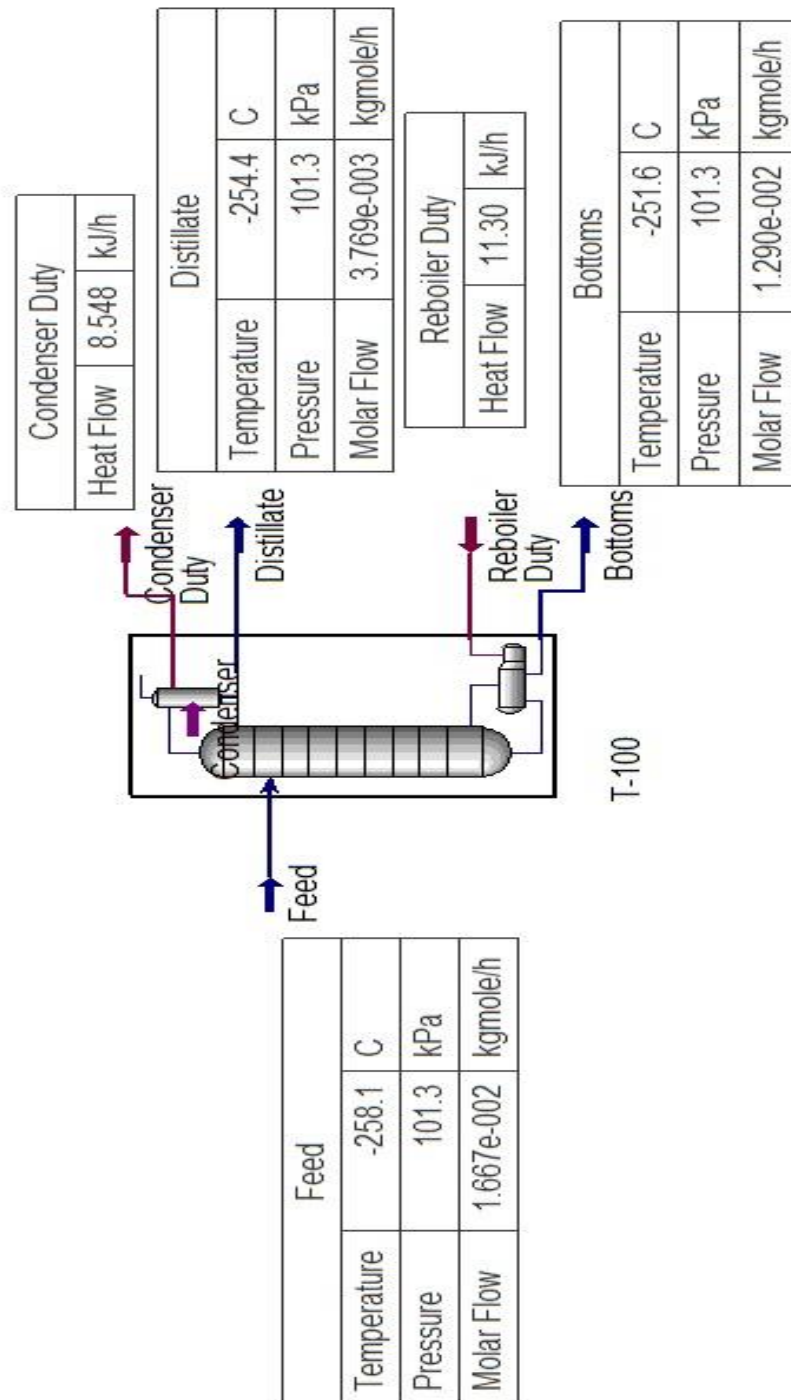


Figure 5.6: Flowsheet of the packed distillation column(15K,400gmole/day)

4. Feed (450 gmole/day)

Table 5.9: Initial Data basis for 450gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.1875
Reflux ratio	1.5
Number of Trays	10
Efficiency	60%

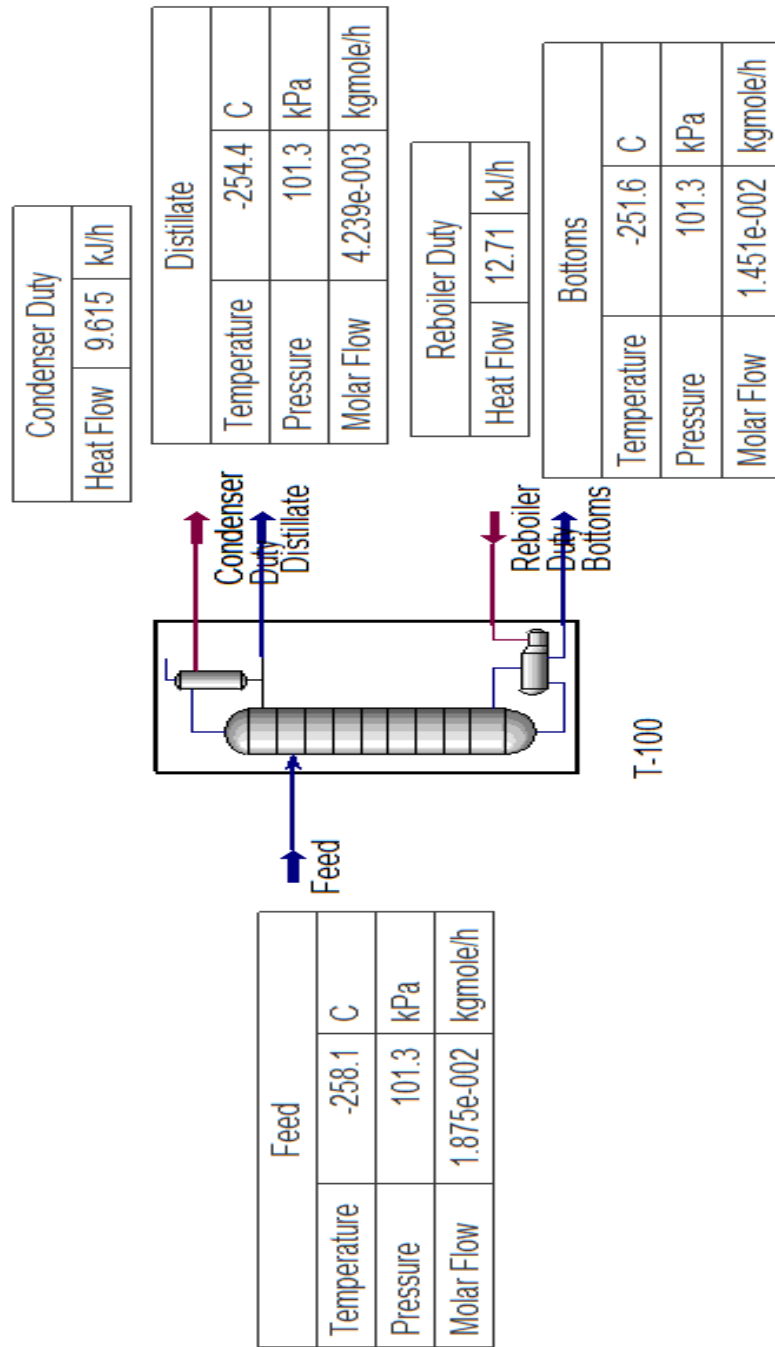


Figure 5.7: Flowsheet of the packed distillation column(15K,450gmole/day)

5. Feed (500gmole/day)

Table 5.10: Initial Data basis for 500gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.020833
Reflux ratio	1.5
Number of Trays	10
Efficiency	60%

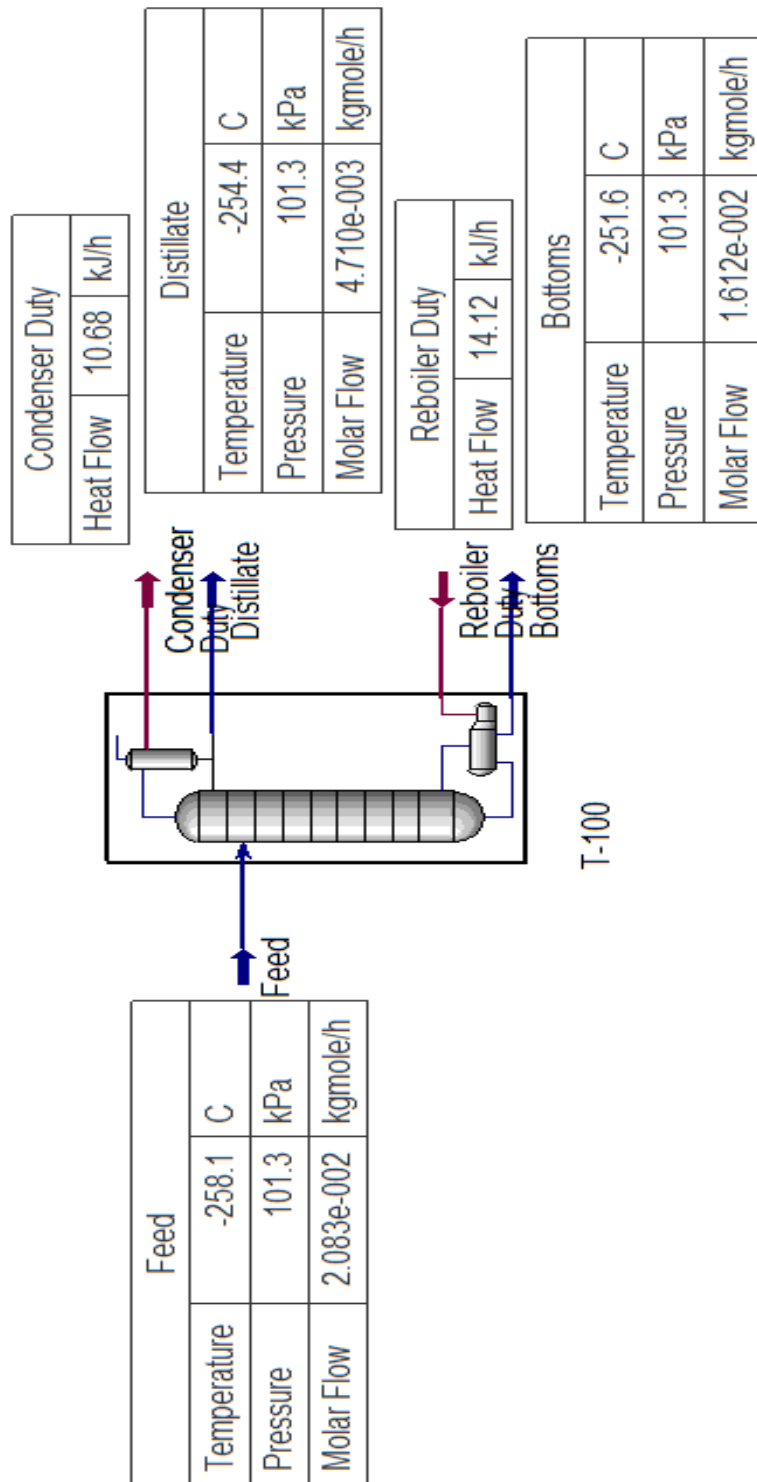


Figure 5.8: Flowsheet of the packed distillation column(15K,500gmole/day)

5.2.2 Saturated vapor ($q=0$, 15K)

1. Feed (300 gmole/day)

Table 5.11 : Initial Data basis for 300gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.0125
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

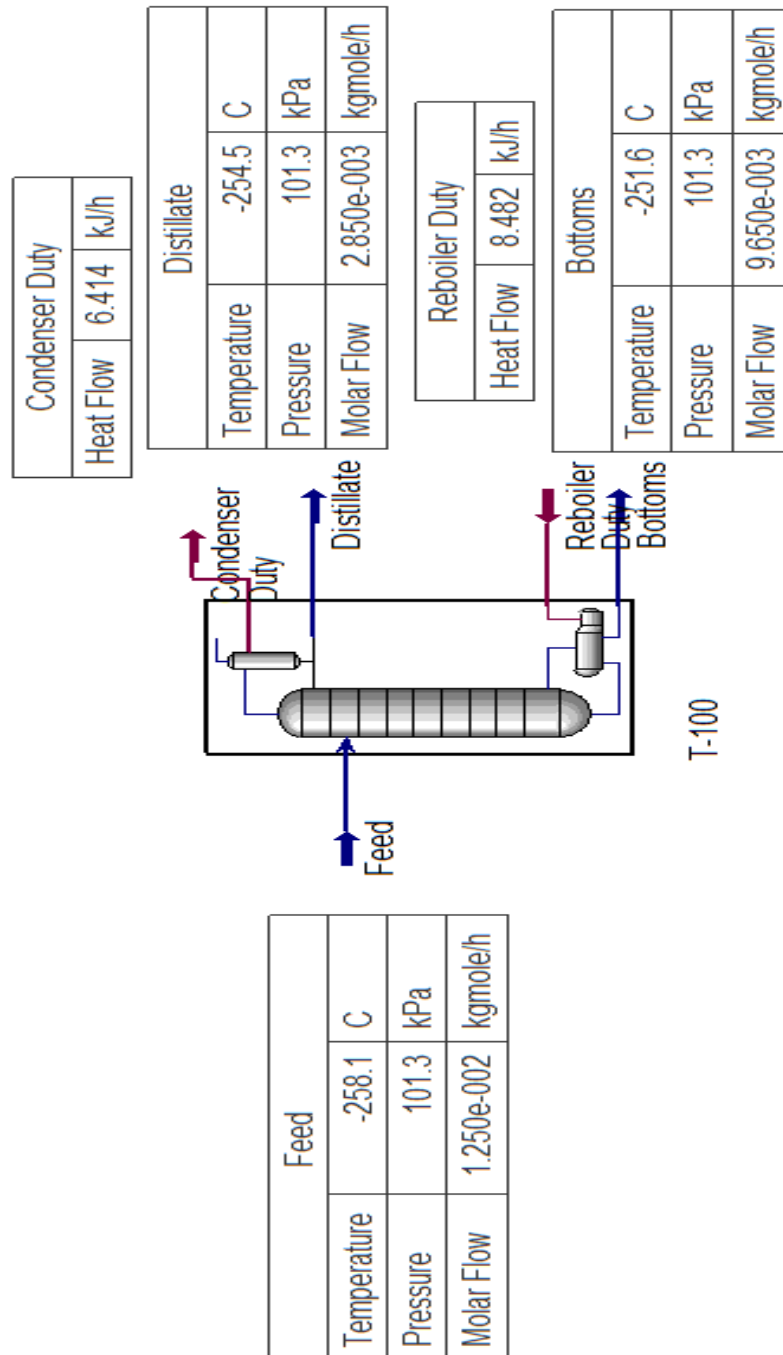


Figure 5.9: Flowsheet of the packed distillation column(15K,300gmole/day)

2. Feed (350 gmole/day)

Table 5.12: Initial Data basis for 350gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.01458
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

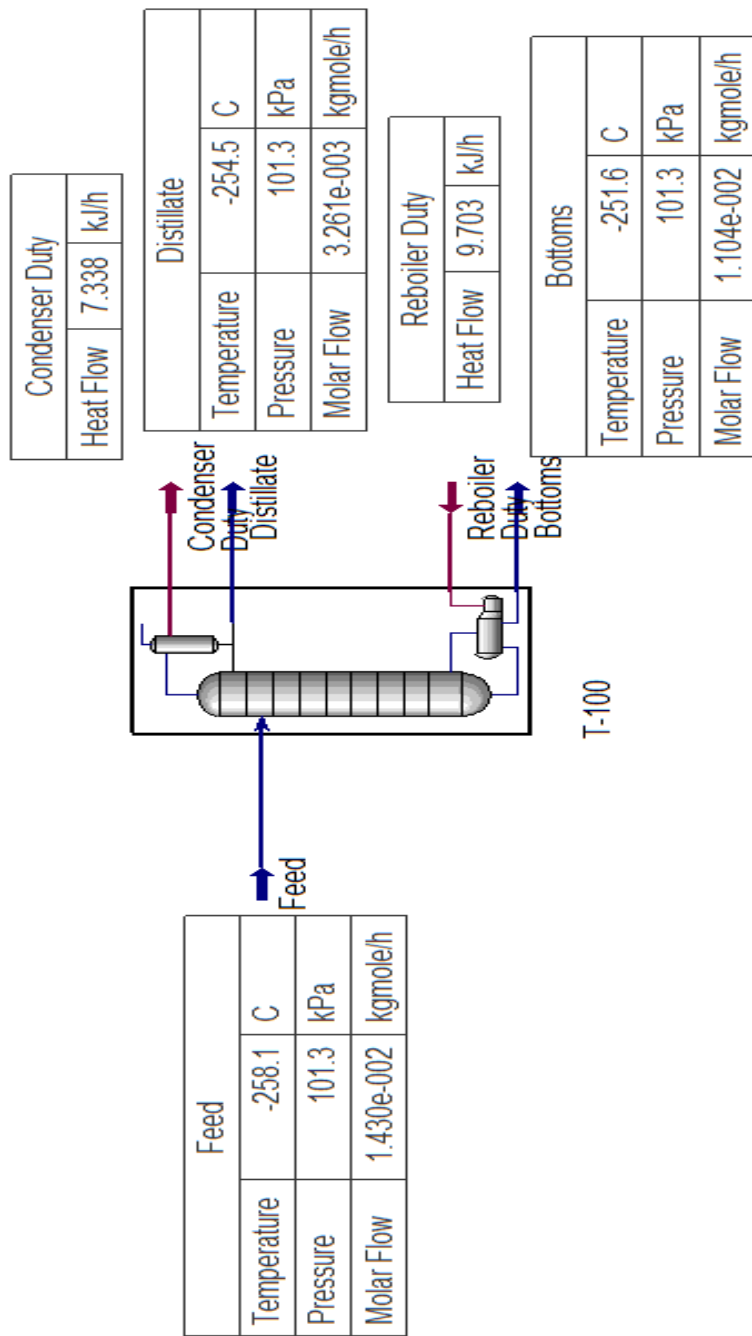


Figure 5.10: Flowsheet of the packed distillation column(15K,350gmole/day)

3. Feed (400 gmole/day)

Table 5.13 : Initial Data basis for 400gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.0166
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

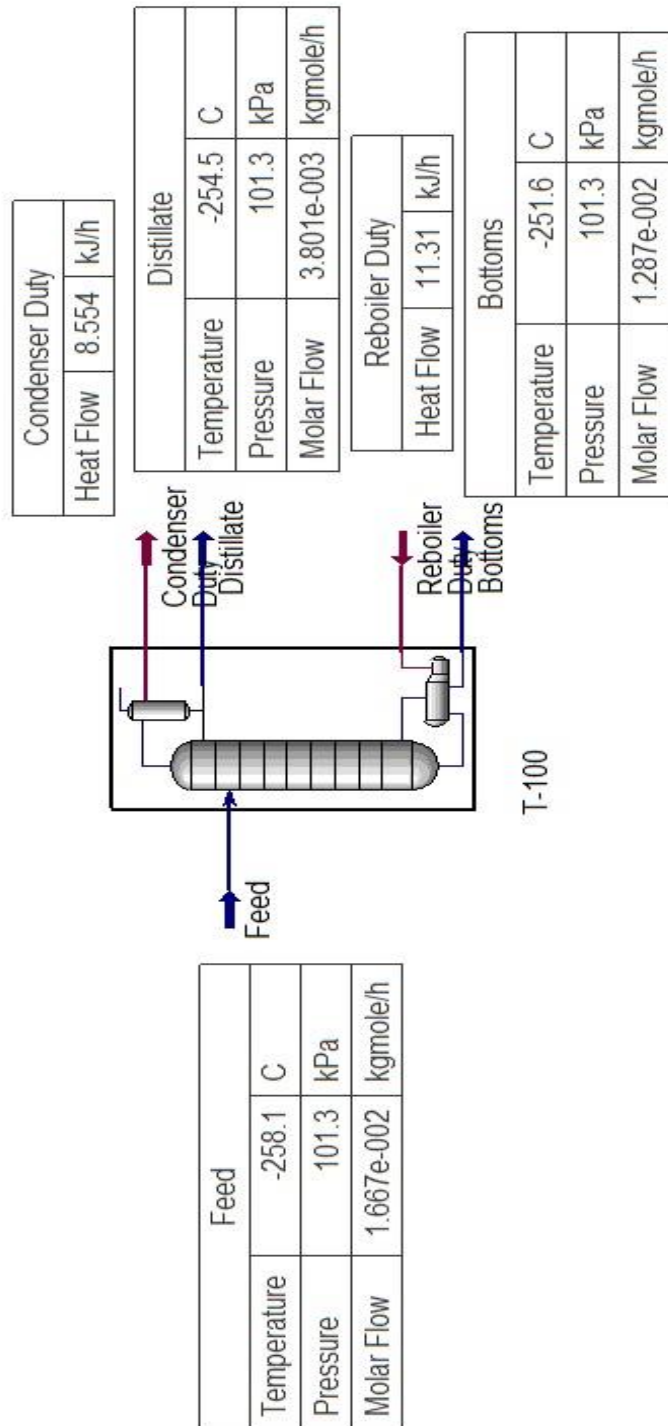


Figure 5.11: Flowsheet of the packed distillation column(15K,400gmole/day)

4. Feed (450 gmole/day)

Table 5.14: Initial Data basis for 450gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.01875
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

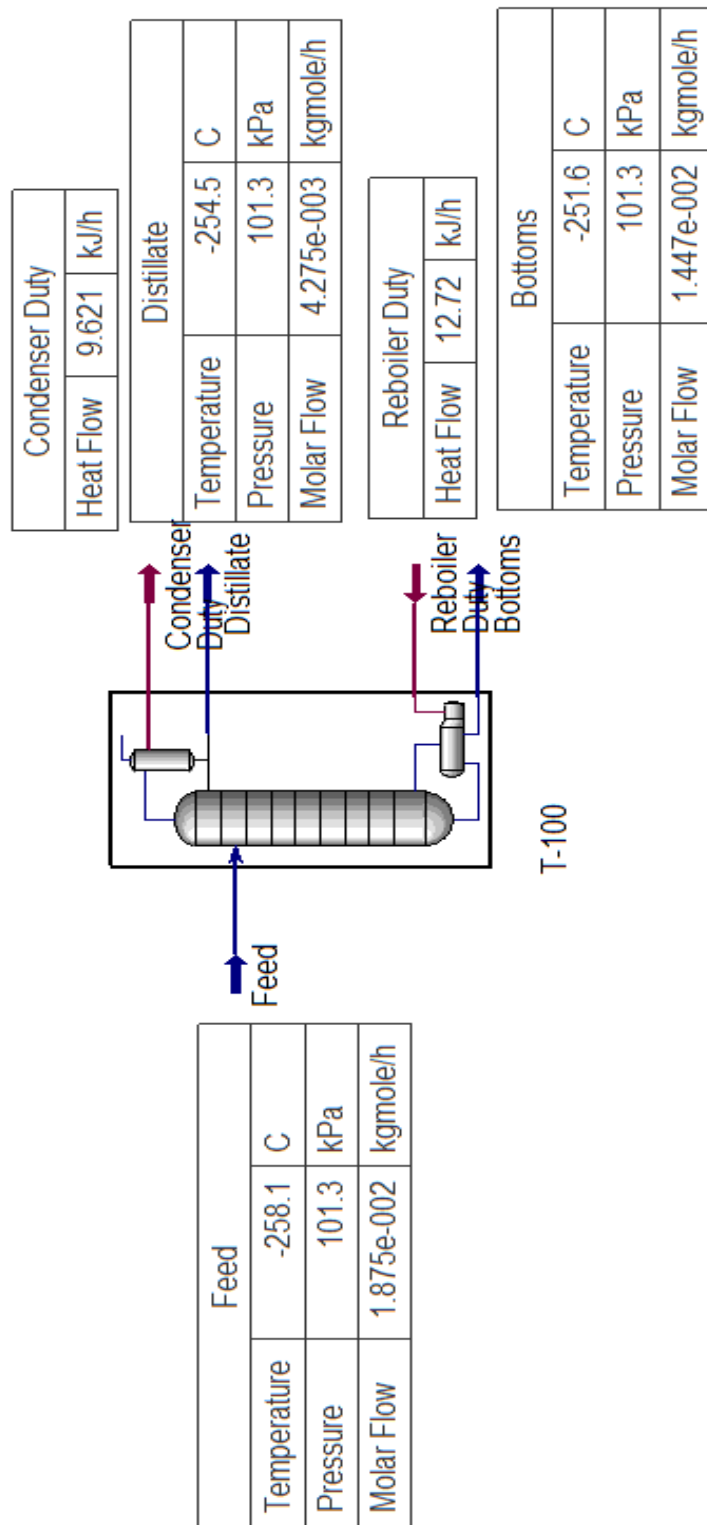


Figure 5.12: Flowsheet of the packed distillation column(15K,450gmole/day)

5. Feed (500 gmole /day)

Table 5.15: Initial Data basis for 500gmole/day and 15k

Feed Inlet Temperature(K)	15
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.02083
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

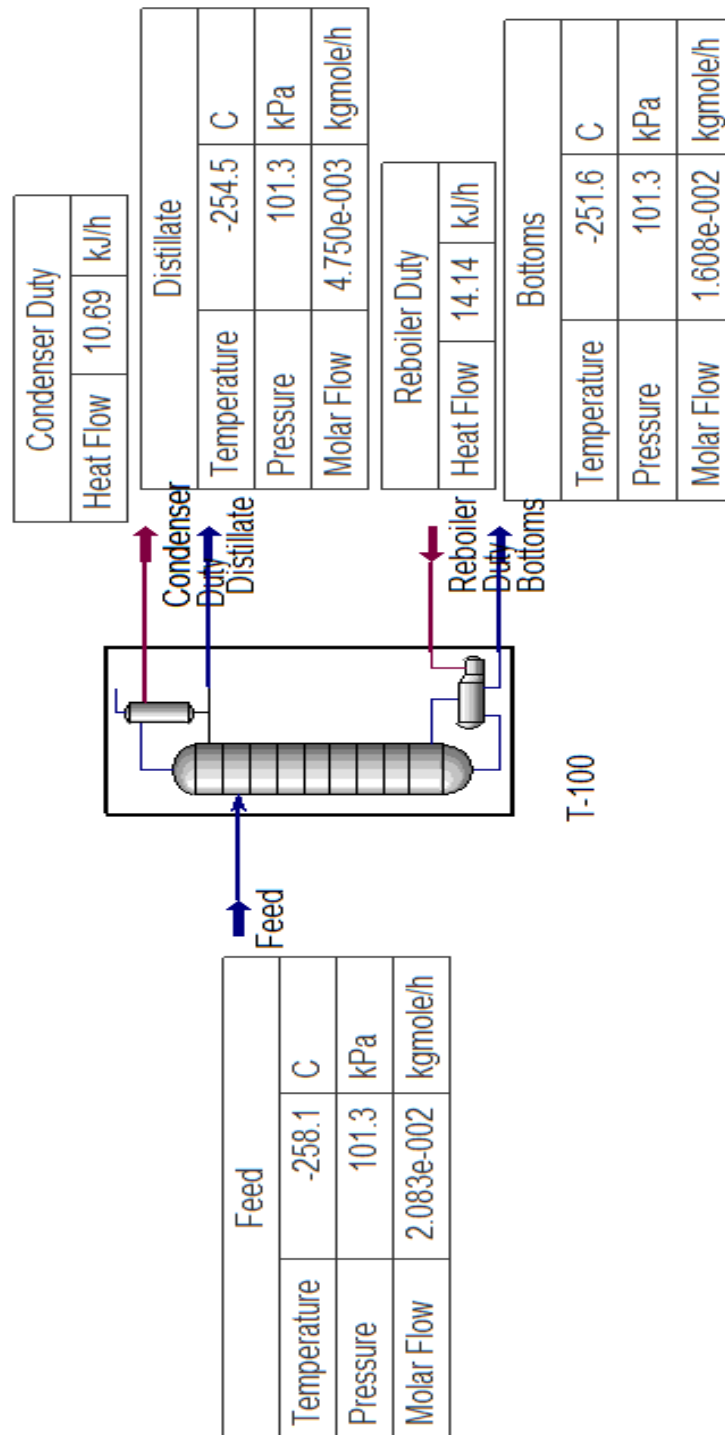


Figure 5.13: Flowsheet of the packed distillation column(15K,500gmole/day)

5.2.3 Saturated Liquid ($q=1$, 16K)

1. Feed (300gmol/day)

Table 5.16: Initial Data basis for 300gmole/day and 16k

Feed Inlet Temperature(K)	16
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.0125
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

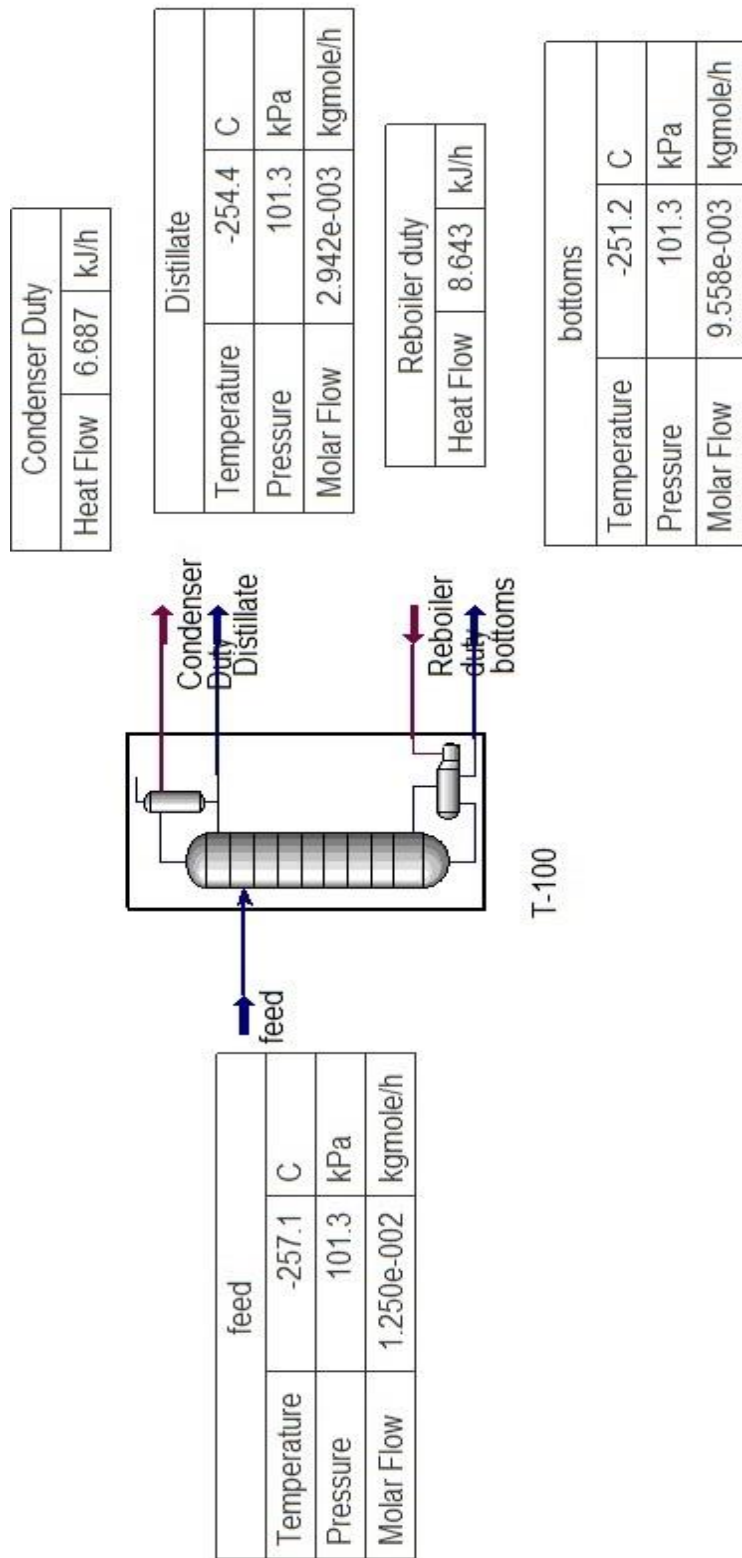


Figure 5.14: Flowsheet of the packed distillation column(16K,300gmole/day)

2. Feed (450 gmole/day)

Table 5.17: Initial Data basis for 450gmole/day and 16k

Feed Inlet Temperature(K)	16
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.01875
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

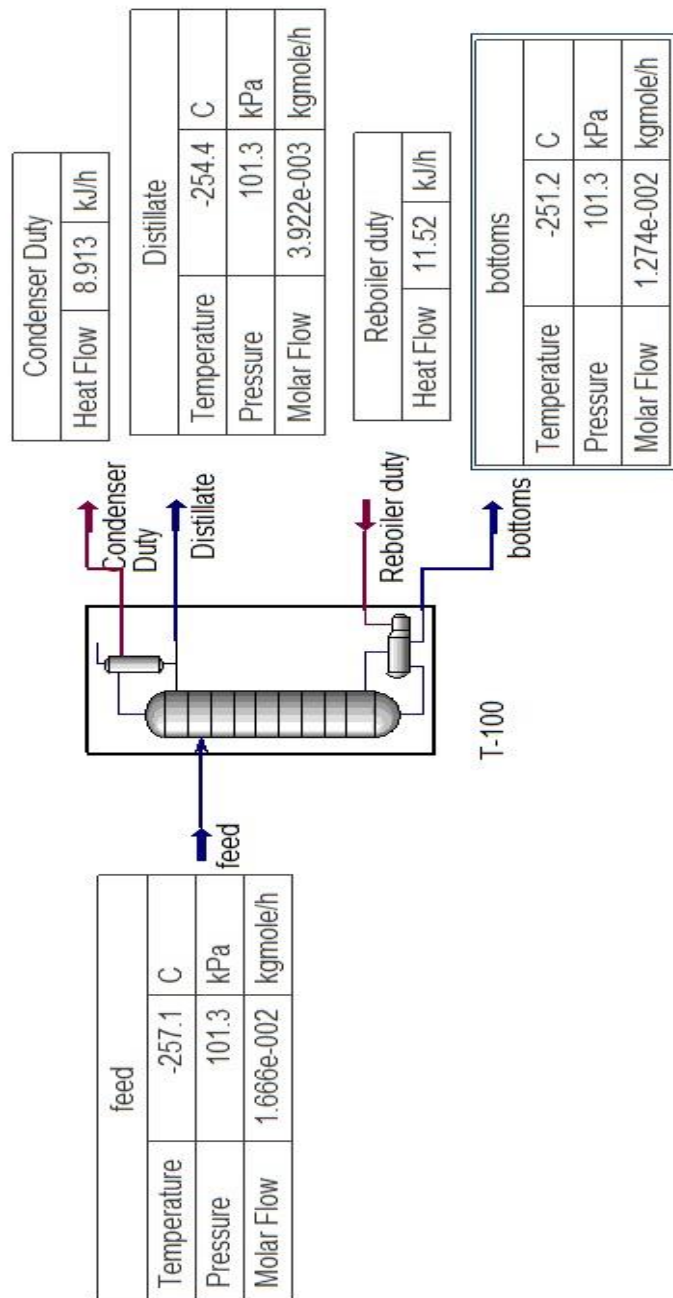


Figure 5.15: Flowsheet of the packed distillation column(15K,450gmole/day)

3. Feed (500gmole/day)

Table 5.18: Initial Data basis for 500gmole/day and 16k

Feed Inlet Temperature(K)	16
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.02083
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

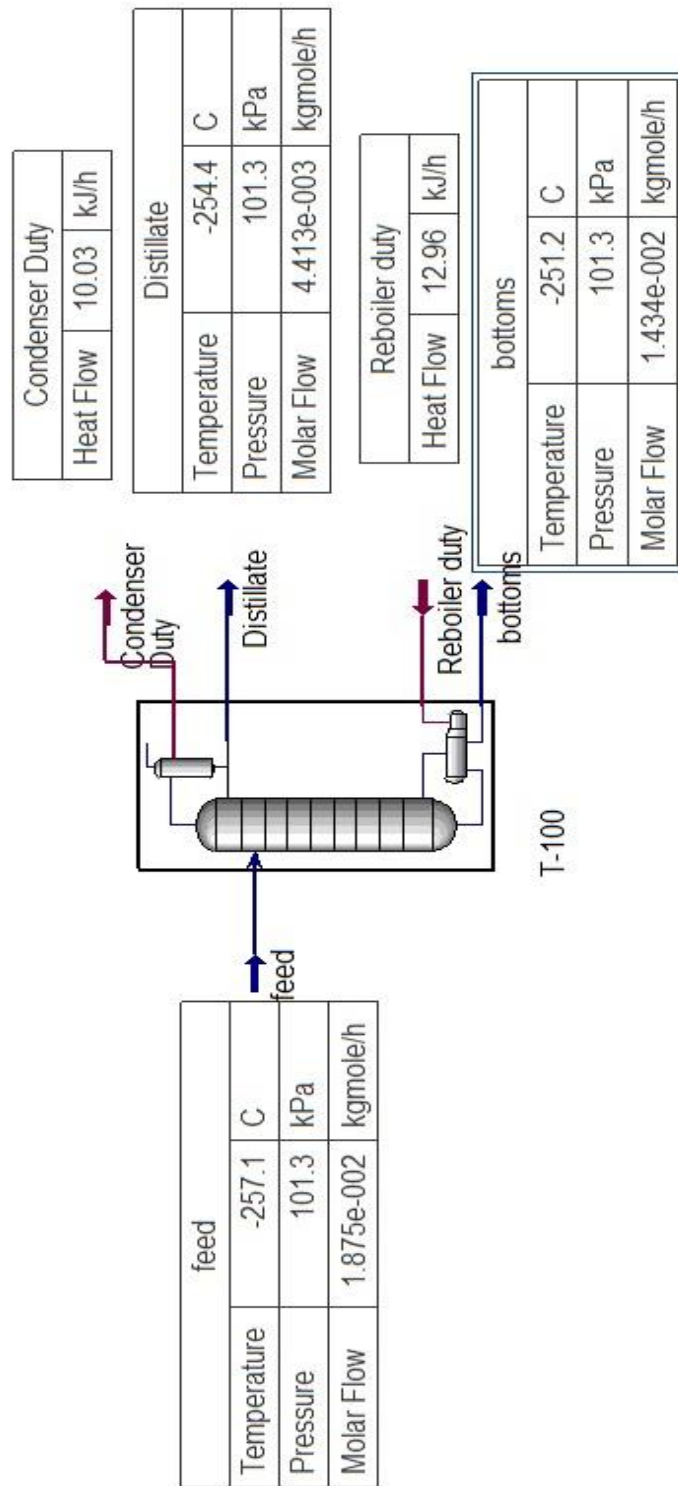


Figure 5.16: Flowsheet of the packed distillation column(15K,500gmole/day)

4.2.4 Saturated vapor ($q=0$, 16K)

1. Feed (300gmole/day)

Table 5.19: Initial Data basis for 300gmole/day and 16k

Feed Inlet Temperature(K)	16
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.0125
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

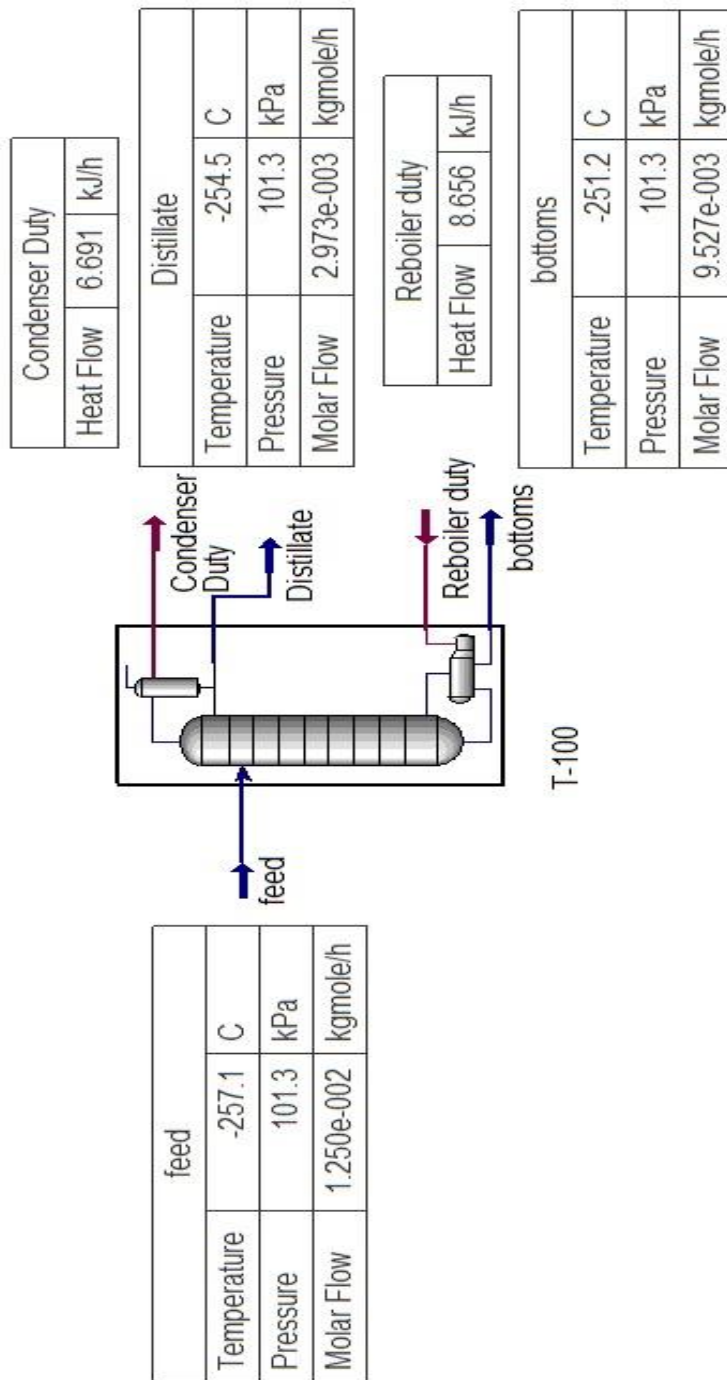


Figure 5.17: Flowsheet of the packed distillation column(16K,300gmole/day)

2. Feed (350gmole/day)

Table 5.20: Initial Data basis for 350gmole/day and 16k

Feed Inlet Temperature(K)	16
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.01458
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

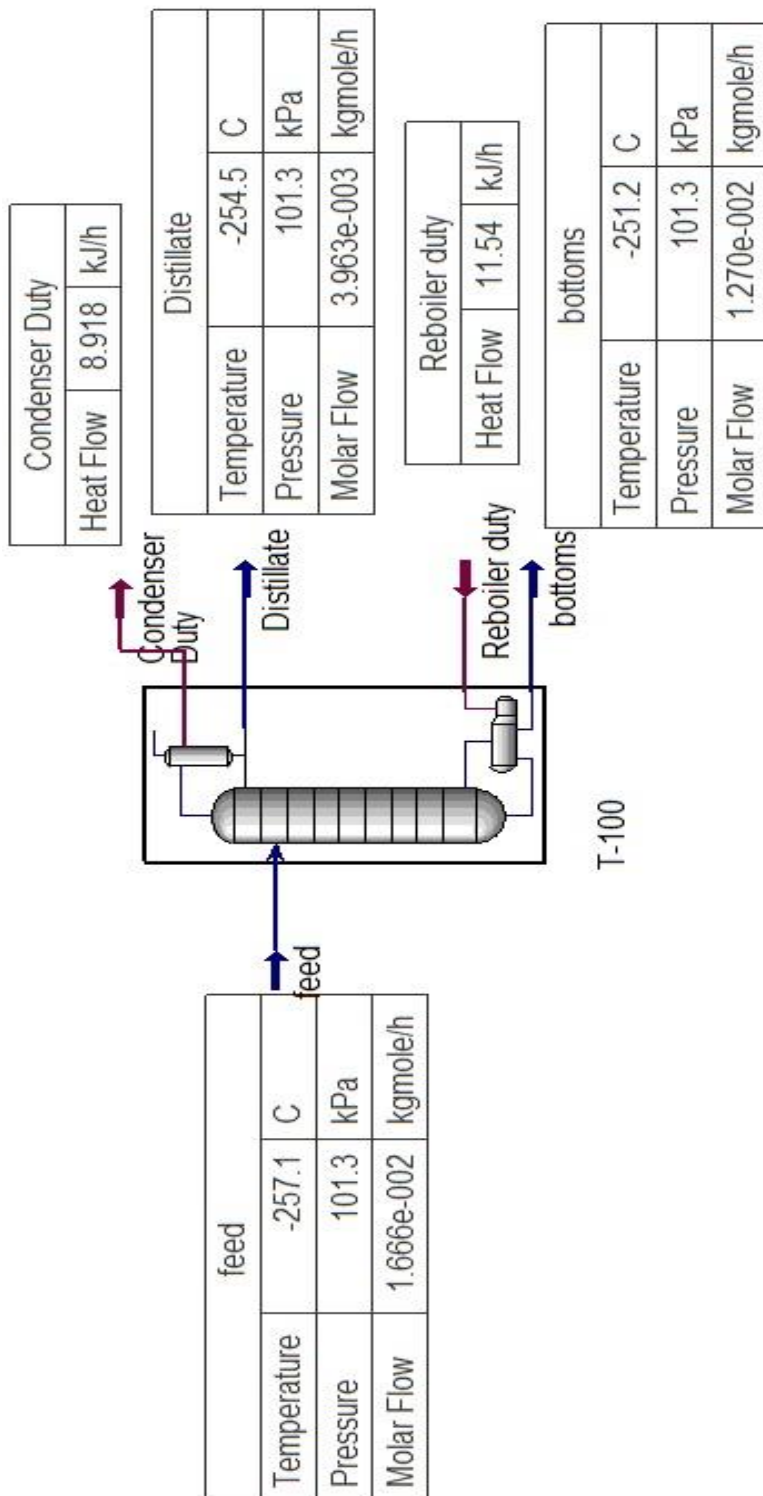


Figure 5.18: Flowsheet of the packed distillation column(16K,350gmole/day)

3. Feed (400gmole/day)

Table 5.21: Initial Data basis for 400gmole/day and 16k

Feed Inlet Temperature(K)	16
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.1666
Reflux ratio	1.5
Number of Trays	10
Efficiency	60%

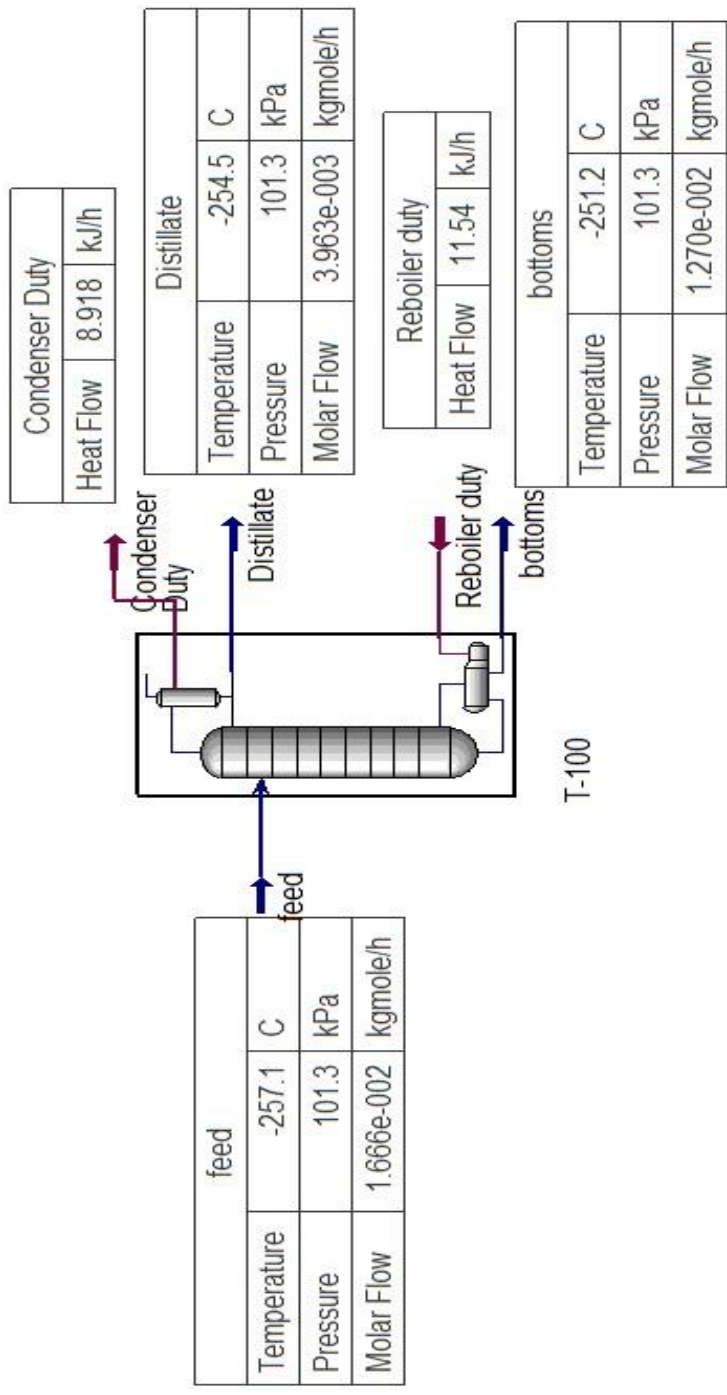


Figure 5.19: Flowsheet of the packed distillation column(16K,400gmole/day)

4. Feed (450gmole/day)

Table 5.22: Initial Data basis for 450gmole/day and 16k

Feed Inlet Temperature(K)	16
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.01875
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

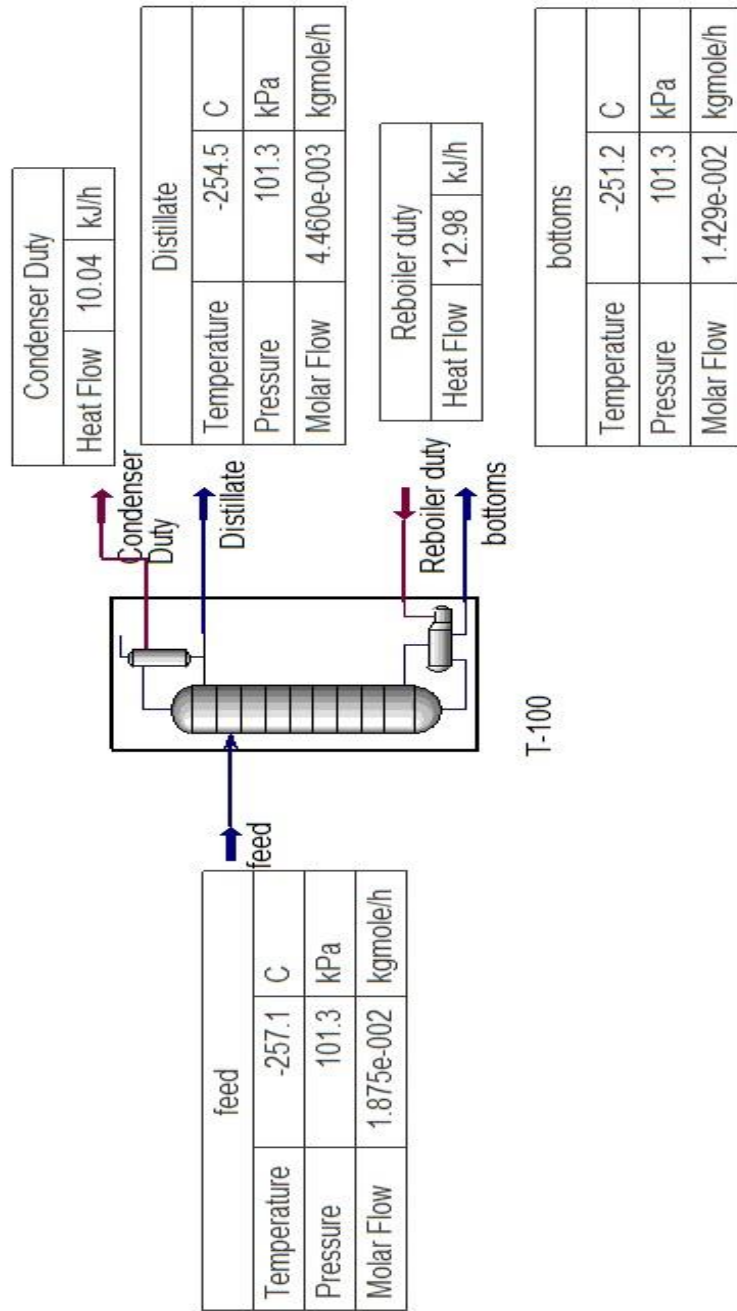


Figure 5.20: Flowsheet of the packed distillation column(16K,450gmole/day)

5. Feed(500gmole/day)

Table 5.23: Initial Data basis for 500gmole/day and 16k

Feed Inlet Temperature(K)	16
Feed Pressure(atm)	1
Feed composition of Hydrogen	0.4
Feed composition of deuterium	0.6
Feed Flowrate(kgmole/h)	0.02083
Reflux ratio	1.5
Number of Trays	22
Efficiency	60%

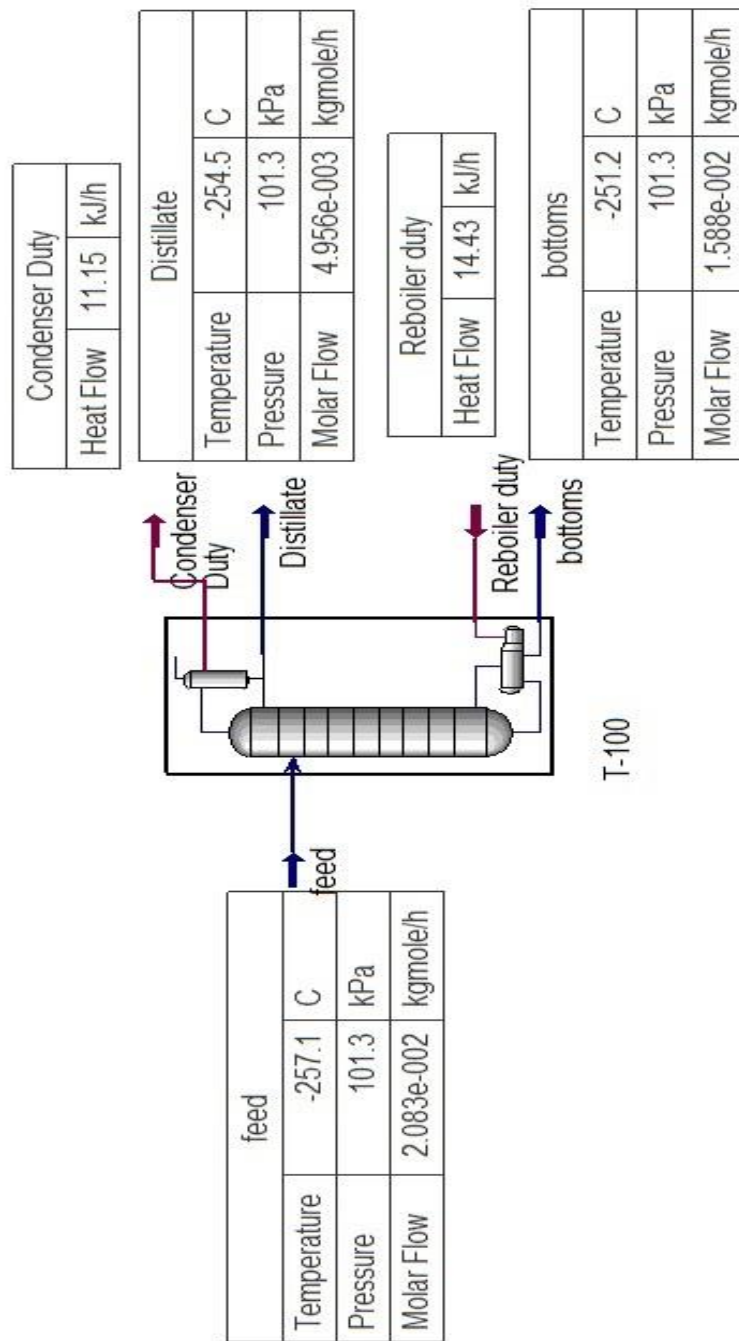


Figure 5.21: Flowsheet of the packed distillation column (16K,500gmole/day)

Chapter 6

Results

Using Aspen HYSYS, we vary the inlet feed flowrate and temperature and we obtain various condenser and reboiler duty. We also determine the distillate and bottom composition of hydrogen and deuterium respectively.

Table 6.1: It is for Saturate liquid, varying the feed flowrate and temperature is 15K

Table 6.2: It is for Saturated Liquid varying the feed flowrate and temperature 16K

Table 6.3: It is for Saturated vapor varying the feed flowrate and temperature 15K

Table 6.4: It is for Saturated vapor varying the feed flowrate and temperature 16 K

1. Saturated liquid (15K)

Table 6.1

Feed(gmole/day)	Condenser Duty (KJ/h)	Reboiler Duty (KJ/h)	Distillate composition of Hydrogen	Distillate Composition of Deteruim	Bottoms composition of Hydroge n	Bottoms composition of Deuteriu m
300	6.414	8.482	0.9882	0.0118	0.2856	0.7144
350	7.33	9.963				
400	8.554	11.31				
450	9.615	12.71				
500	10.68	14.12				

2. Saturated Liquid (16K)

Table 6.2

Feed(gmole/day)	Condenser Duty (KJ/h)	Reboiler Duty (KJ/h)	Distillate composition of Hydrogen	Distillate Composition of Deuterium	Bottoms composition of Hydrogen	Bottoms composition of Deuterium
300	7.541	9.541	0.9849	0.0151	0.2191	0.7801
350	7.801	10.08				
400	8.913	11.52				
450	10.03	12.96				
500	11.15	14.40				

3. Saturated Vapor(15K)

Table 6.3

Feed(gmole/day)	Condenser Duty (KJ/h)	Reboiler Duty (KJ/h)	Distillate composition of Hydrogen	Distillate Composition of Deuterium	Bottoms composition of Hydrogen	Bottoms composition of Deuterium
300	6.414	8.482	0.9998	0.0002	0.2804	0.7196
350	7.338	9.703				
400	8.554	11.31				
450	9.621	12.72				
500	10.69	15.14				

4. Saturated Vapor(16K)

Table 6.4

Feed(gmole/day)	Condenser Duty (KJ/h)	Reboiler Duty (KJ/h)	Distillate composition of Hydrogen	Distillate Composition of Deuterium	Bottoms composition of Hydrogen	Bottoms composition of Deuterium
300	6.691	8.656	0.9998	0.0002	0.2804	0.7196
350	7.807	10.10				
400	8.918	11.54				
450	10.04	12.98				
500	11.15	14.43				

With the above tables, we plot the composition vs Tray position graph for the various number of trays. From this graph, it shows us the mole fraction of the component at various tray position

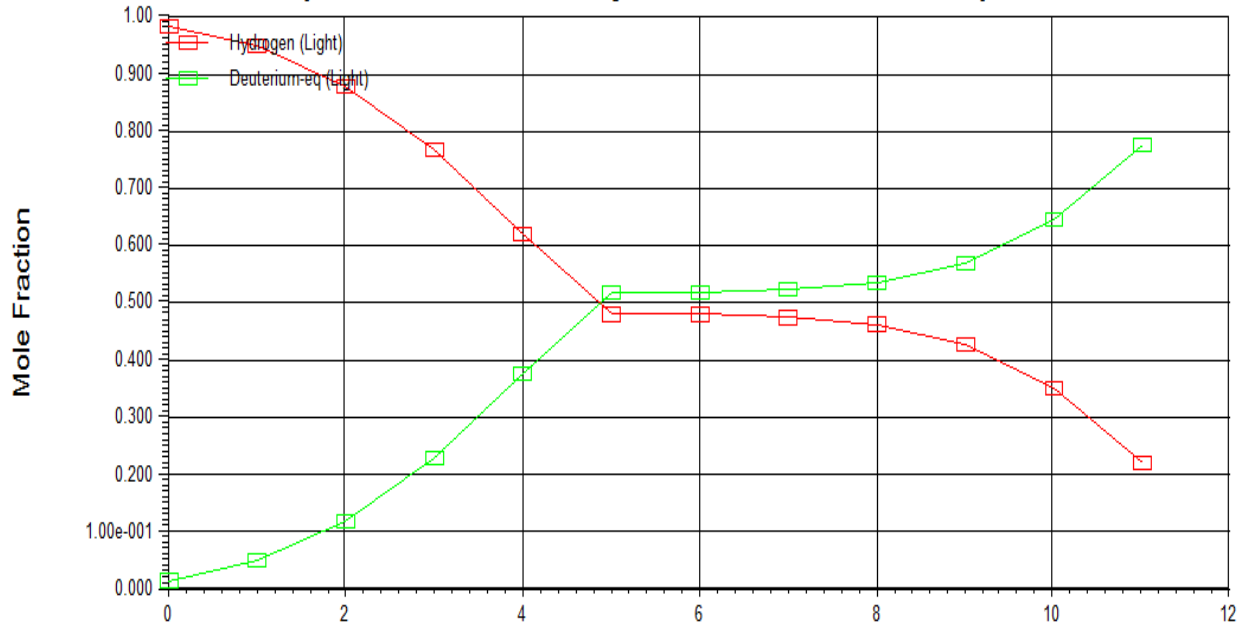


Figure 6.1: Composition Vs Tray position for saturated liquid(10 stages)

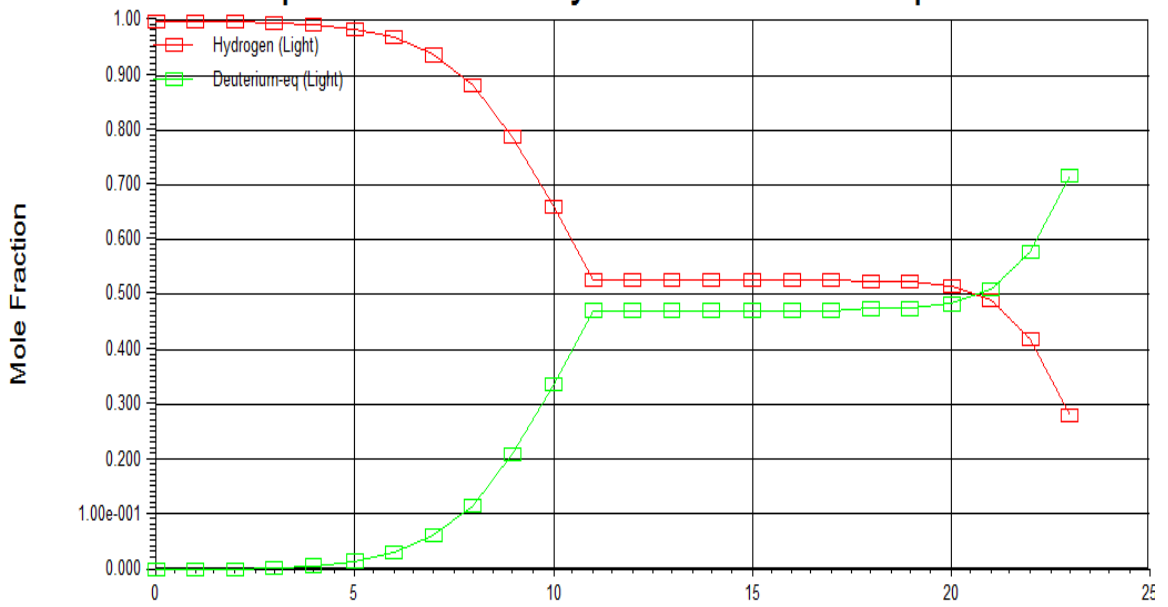


Figure 6.2: Composition Vs Tray Positions for saturated vapor (22 stages)

Diameter and Height of the column

With help of the simulation software Aspen HYSYS, we can determine the various height and diameter of the column. In the below table, we have compared between the Saturated liquid and Saturated vapor. We have also seen that structured packing gives us a compact structure. The efficiency of the structured packing is higher than the other packing methods.

Saturated Liquid	Diameter(m)	Height(m)
Random Packing (Intalox Saddles 1 inch)	0.3048	3.048
Structered Packing (Koch-Sulzer)	0.1524	1.524

Saturated Vapor	Diameter(m)	Height(m)
Random Packing (Intalox Saddles 1 inch)	0.3048	6.706
Structered Packing (Koch-Sulzer)	0.1524	3.353

Chapter 7

Conclusion

The project presents an unsteady state mathematical model for performance simulation of a cryogenic distillation column for hydrogen isotope separation. Evaluation of some of the most important parameters of column hydraulic behavior has also been carried out using data from literature. Increasing feed flow rate affects the time required to attain the steady state but does not affect the final top and bottom product compositions achieved. The distillation column model presented here can be used as a method of solving the more difficult column design problem through the ‘design by repeated simulation’ philosophy, by varying some of the parameters. It may further be integrated with models of the cryogenic refrigeration cycle (to which it will provide calculated values of the heating and cooling duty inputs from the reboiler and condenser duties) and it can also be used to provide necessary inputs to energy integration studies to minimize energy requirements for the cryogenic systems. Prediction of separation factors for this distillation, considering an equation of state model to account for non-idealities. We have seen that structured packing gives us an efficient structure.

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