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Capital Cost Evaluation for Optimum Process Design of Cryogenic Air Separation

Diploma Thesis
by
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Nomenclature

$\dot{e}_{ij}$	Energy flow of to equipment i from energy carrier j	$[kW]$
$\dot{m}_i$	Mass flow of component i	$[\frac{kg}{s}]$
C_B^i	Reference cost of equipment i	[\$]
C_E^i	Cost of equipment i	[\$]
C_{EC}^i	Mass specific cost of energy carrier i	$[\frac{\$}{kW}]$
C_{RM}^i	Mass specific cost of raw material i	$[\frac{\$}{kg}]$
C_1	Reference equipment cost at time 1	[\$]
C_2	Reference equipment cost at time 2	[\$]
C_P	Total process cost	[\$]
C_P^0	Reference process cost	[\$]
C_{EC}	Total cost of energy	[\$]
C_{RM}	Total cost of raw materials	[\$]
f_C^i	Design complexity correction to equipment cost	$[-]$
f_M^i	Material selection correction to equipment cost	$[-]$
f_P^i	Pressure correction to equipment cost	$[-]$
f_T^i	Temperature correction to equipment cost	$[-]$
I_1	Cost index at time 1	$[-]$
I_2	Cost index at time 2	$[-]$
M^i	Equipment specific factor	$[-]$
N_E	Number of equipment pieces in the process	$[-]$

N_{RM}	Number of raw materials	$[-]$
Q^i	Specific quantity for equipment i	$[variable]$
Q^i_B	Equipment specific reference quantity	$[variable]$
Q_P	Process capacity	$[\frac{kg}{h}]$
Q^0_P	Reference process capacity	$[\frac{kg}{h}]$
t_{op}	Time of process operations	$[s]$
x	Degression coefficient	$[-]$

1 Introduction

Air separation technology, or – more generally speaking – gas separation technology, lies at the heart of the modern process industry. Highly pure oxygen and nitrogen ore uses in many industrial applications. Modern power generation processes, such as the currently developed OXICOAL process, rely on incineration with pure oxygen to produce flue gases with very high carbon dioxide content for further storage. Nitrogen is essential to many widely used processes such as the production of ammonia in the Haber-Bosch synthesis, as fertilizer or in many organic reactions.

2 Air separation technology

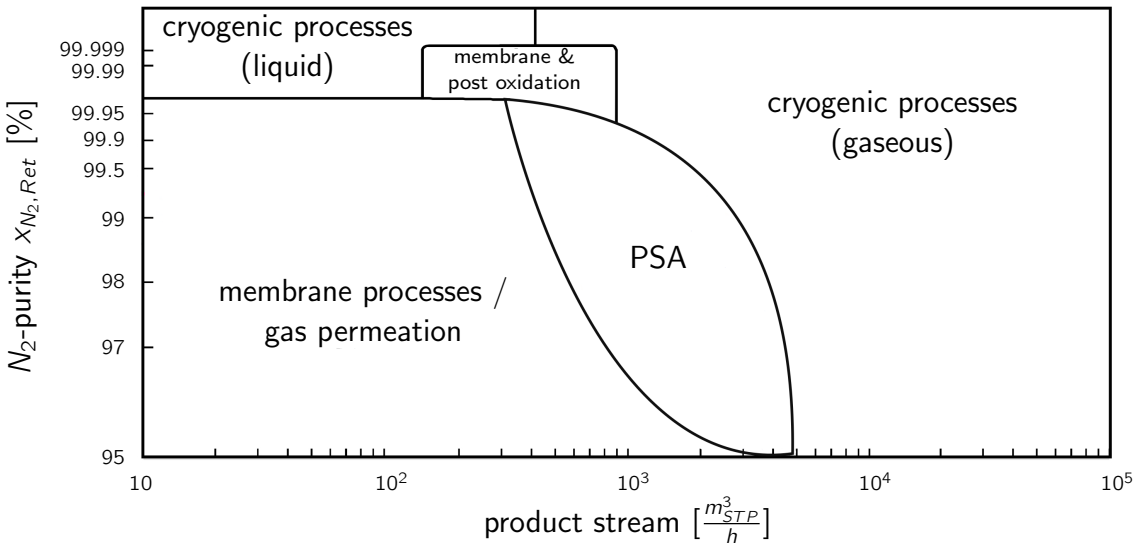

Figure 2.1: Comparison of Air Separation Technologies [4].

There are several ways besides cryogenic air separation that can be employed to separate gas mixtures. In this chapter different competing technologies and their main applications will be discussed. The predominately used technologies are cryogenic distillation, pressure swing adsorption (PSA) as well as gas permeation (GP). In the distillation process the gas is first liquefied. Separation is the achieved by the different concentration differences in vapor and liquid phase. PSA relies on the different affinities of gaseous species to adsorb to certain materials in order to extract a component form a mixture. During gas permeation membranes are used. Each species migrates in different quantities through a given membrane depending on process parameters and membrane structure.

fig. 2.1 illustrates the most economically viable processes depending on product purity and product stream volume. It can be seen that alternative air separation processes cannot supply the high quality or quantity of the cryogenic process. Due to that cryogenic air separation is thought to be the main supplier of highly pure gases in industrial quantities for years to come [1]. The alternative processes however offer some very appealing characteristics, which make them the favorable choice when lower quantities of product or more moderate purity is required. The cryogenic process is always connected with an considerable energy consumption for the liquefaction and compression. Due to that smaller implementations of the process a very unlikely to yield economically sound solutions to a separation problem.

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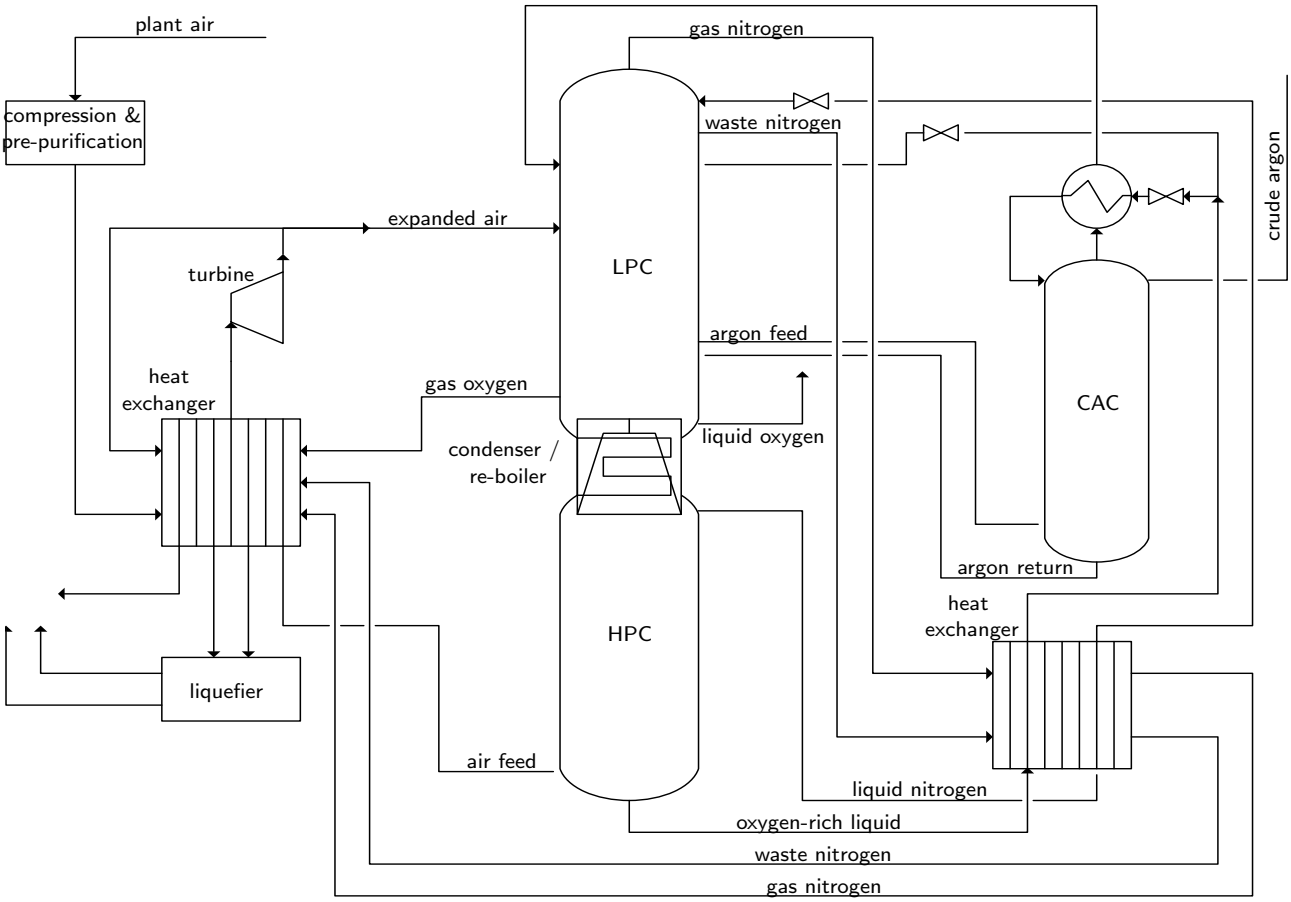

Figure 2.2: Schematic representation of the cryogenic air separation process.

2.1 Cryogenic air separation

Cryogenic Air Separation finds applications over a great variety of industries among others refining, petrochemicals, medical, food & beverages and environmental [5]. Furthermore prospective processes for power generation from fossil sources in form of the integrated gaseous combined cycle (IGCC) integrates the air separation process in order to enable more environmentally friendly power generation [2].

As can be seen in fig. 2.2 double effect heat integrated distillation column lies at the heart of the air liquefaction processes. It consists of a high pressure column (HPC) operating at 0.68 MPa and temperatures below 130 K as well as a low pressure column (LPC) which operates at around 0.13 MPa an comparable temperatures. In order to also attain highly pure argon as a product the process may also include a crude argon column (CAC) which works at slightly lower pressures than the LPC.

The plant air entering the process is initially purified, where carbon and nitrogen oxides as well as solid contaminants are removed, and then compressed to process conditions. The compressed air is then cooled against product streams namely liquefied nitrogen, oxygen and argon. The air stream is then divided into several sub-streams. One of those is fed into the HPC bottom, while another is expanded by means of a turbine and further cooled down through the Joule- Thompson effect. Aside from further cooling energy from the initial compression is thus partially recovered. This expanded air stream is then fed into the LPC. At the bottom of the LPC liquid as well as gaseous oxygen are

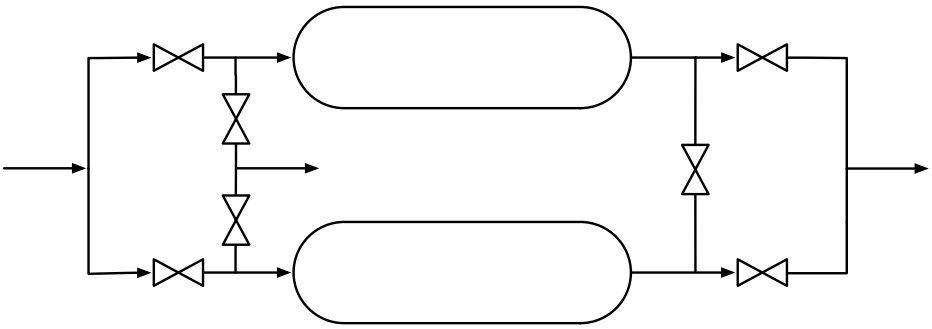

Figure 2.3: Schematic representation of the PSA process.

recovered as desired products. The bottom and top streams from the HPC are made up of an oxygen rich liquid as well as liquid nitrogen. The liquid nitrogen stream is led though an heat exchanger an the fed as reflux into the top of the LPC. The bottom stream is, after heat integration, partially fed into the LPC as well as CAC. From the lower part of the LPC a side stream is drawn and led into the bottom of the CAC. At the same point the reflux from the CAC is fed back into the LPC [6].

2.2 Pressure swing adsorption

Pressure Swing Adsorption has been employed to separate gaseous mixtures for some time. During the 80's and 90's commercial applications for the production of oxygen or nitrogen have gained more and more attention. Especially the ability to construct very compact units the size of a briefcase, have led to the implementation of PSA processes for treatment of asthma patients or other medical appliances. But also larger scale plants have successfully been utilized, for example in the paper industry during the de-lignation of pulp. It remains true however, that for large scale industrial settings with high product quality demands, cryogenic separation remains the most viable alternative.

Separation is achieved during the PSA process by adsorption of one component in the mixture to a given bed. Once the bed is saturated with a the adsorbing species, it has to be regenerated in order to continue production. The ability to adsorb a certain species is dependent on the system pressure. At higher pressures more gas can be adsorbed then at lower pressures. Thus by reducing the pressure in the reaction vessel, the Adsorbent can be regenerated.

In order to avoid non-continuous processes, two or more reaction vessels are employed. Therefore the saturated vessel can be regenerated, while the other one continues production. By alternating adsorption and regenerating in the different vessels continuous production can be achieved. A schematic for a simple two bed cycle is shown in fig. 2.3. Ambient air is first led through the first reaction vessel at the elevated pressure. Within the vessel nitrogen is adsorbed until saturation is reached. At that point the ambient air is led through the second vessel. A fraction of the product stream is fed into the first vessel and used as sweep for the regeneration of the adsorbent at lower pressure.

Depending on the size of the process two different pressure level are used. One cycle adsorbs the nitrogen at a pressure of approximately 7.5 bar while regeneration is done at ambient pressure. Within

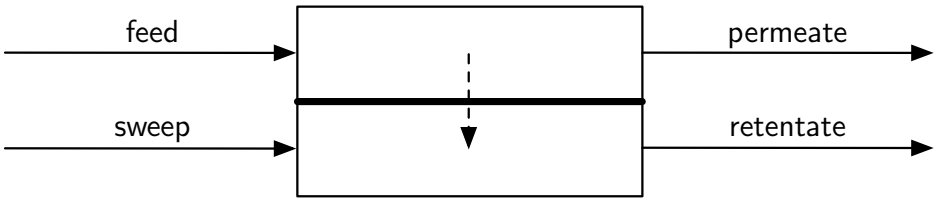

Figure 2.4: Gas permeation process.

the alternative approach adsorption occurs under ambient condition, while for the regeneration step a vacuum pump reduces the vessel pressure. This process is the called Vacuum Pressure Swing Adsorption (VPSA).

An important role when designing the product is the choice of the adsorbent. For almost all current applications of PSA alumosilicates or zeolithes have been designed, tailored to the specific separation task. Their main advantages include a high selectivity towards a specic gas to be adsorbed as well as a very homogenous distribution of diameters in the molecular sieve.

2.3 Gas permeation

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The separation of mixed gases by membrane process is called gas permeation. Its main strength in comparison with alternative processes are the low energy consumption and the possibility to produce flexible mobile units. As mentioned before it is not however capable of producing high quantity highly pure product streams. As fig. 2.1 illustrates the main application for the gas permeation process are small to moderate product streams at intermediate purities.

fig. 2.4 shows the schematic for a single stage membrane unit. Within the feed stream the gaseous mixture is fed into the unit, which can quickly be implemented. Within the unit one or more species migrate favorably through the membrane. In this case mostly dense polymer membranes are employed used. There have been some impressive results with metallic membranes, but due to the very high material costs they have not been adapted by the industry. Furthermore, since gaseous phases often have rather small molecular species, porous membranes cannot achieve desired separation. The driving force the separation process is a difference in partial pressure or species activity across the membrane. According to the molecular structure of each species, the structure of the separating membrane as well as the process parameters pressure and temperature, they permeate through the membrane in different quantities.

The process of permeation can be subdivided into three separate steps. Sorption at the membrane / feed interface, diffusion through the mostly dense polymer membrane and finally desorption at the permeate side of the membrane.

3 Process design

Once a particular reaction or production sequence has been developed in a laboratory it needs to be scaled up to produce the desired product in quantities large enough to meet market demand to a price that allows competative prices. This is where process design comes into play. At the begin of the design process often only the raw material as well as the desired products, along with the necessary chemical reactions are specified. It is then the task of the process engineer to find a series of production steps which lead to the production of this product. Each step denotes a specific function and the connected functions form a process. At the end each specific function has to be assigned a specific technical realization.

Usually there are numerous options available to perform certain tasks and in order to be realized any endeavor will need to yield acceptable profits. Different options will therefore have to be compared from an engineering and an economic standpoint alike. For complex processes the amount of possible options becomes enormous. Too many to be manually examined and evaluated.

Number of options for separation problem – ref douglas

Process Engineers have to rely on heuristics to limit the number of options and identify the most promising candidates for further studies. These candidates can then be compared in terms of economic performance. In order to do so one has to rely on simulation studies and experiments. As experiments and the construction of pilot plants are very costly the aim is to minimize those. WIth the rise in available computing power the numerical simulation of processes has become a very powerful tool to support the design process and has the ability to replace numerous experiments. Not only can possible options be evaluated but also can optimal process configurations from a limited pool of options be generated.

To conduct simulation studies first a process model needs to be created. This models in its most general case is a set of partial differential and algebraic equations. When formulating the model great care needs to be applied, as any simulation study can only be as accurate as the underlying model. The process engineer is faces with the task to find an adequate representation of the physical system which delivers meaningful results within an reasonable amount of time. Further enhanced is this problem when the model is to be used in model predictive control, where (approximate) solutions of complex systems might need to be available within seconds or fractions of a second.

3.1 Process model

4 Process economics

Aside from question wether a certain process is capable of producing products according to its specifications, it needs to be investigated if it does so in an economically viable manner. The modeling of process economics is a powerful tool to estimate project profitability. The evaluation of process economics has three major aims in the design phase.

- Compare design options with regard to profitability.
- Economically optimize a given design.
- Estimate project profitability

In any case the total cost of the project as well as the cash flow structure will have to be analyzed to supply an accurate estimate of the economic conditions. Furthermore an adequate measure to compare and analyze a project in economic terms needs to be employed.

The following sections will first describe how to estimate the total project cost in different stages of the design process. It is evident that, as the more information about a given process becomes available, the accuracy of any cost estimate will increase as well. During the design phase of a process roughly three different stages of cost estimation can be formulated.

- An estimate before designing the process yields an order of magnitude estimation for supporting market research efforts. Error $> 30\%$
- Estimate in the early design phase based on essential process equipment. Error $\pm 30\%$
- Estimate based on an advanced flowsheet and relevant process parameters. Error $\pm 20\%$

Once detail engineering commences, even more accurate calculations with errors reducing to $\pm 5\%$ can be undertaken[3]. At that point a concrete process option will have to be chosen and the investment decision will already have to be made. All optimization measures within the scope of this thesis will have concluded at that time.

Within sec. 4.1 first we will take a look at how the total cost of a chemical process might be estimated at different design stages. Subsequently in sec. 4.2 the different ways of evaluating a certain investment options and estimating a projects profitability will be discussed.

4.1 Project cost

An important factor in every given project is the total cost. During the design of a chemical process many important aspects of the future cost structure are unknown, as the final design is in development.

In general the total cost of implementing and operating a production site can be broken down into several subcategories.

- Battery limit investment
- Utility investment
- Off-Site investment
- Engineering fees
- Working capital

4.1.1 Before process design

Before any details about the process to be implemented are known, an estimate can only give an order of magnitude towards cost to be expected. The cost of the new process C_P can be related to the cost of a reference process C_P^0 by

$$C_P = C_P^0 \cdot \left(\frac{Q_P}{Q_P^0}\right)^x. \tag{4.1}$$

The degression coefficient x needs to be correlated from historical data.

As the overall price structure will change over time, the reference price will not reflect the current market situation. In order to adjust for that shortcoming several price indices are published all over the word. Some of those tailor to special branches of the industry, others give a picture of the price-development in a economy as a whole. The price ration of the prices at different times will then be equal to the ration of the price indices at the respective times

$$\frac{C_1}{C_2} = \frac{I_1}{I_2}. \tag{4.2}$$

For each index an somewhat arbitrary reference year is chosen. Among the most common indices are the Marshall & Swift index, the Nellson-Farrar-Index or the Chemical Engineering index. Some exemplary values for these indices are given in tab. 4.1. As one can see the development within the process industry very well matches the development in the economy as a whole, which is why for this rough estimate general indices should suffice.

4.1.2 During process design

Once the future design has been has been broken down to fewer potential options and first process flowsheets are available a more elaborate approach becomes possible.

	Marshall & Swift Installed Equipment Index 1926 ≡ 100		Nelson-Farrar Refinery Construction Index 1946 ≡ 100	Chemical Engineering Plant Cost Index 1957 ≡ 100
year	all industries	process industry		
1975	444	452	576	182
1980	560	675	823	261
1985	790	813	1074	325
1990	915	935	1226	358
1995	1027	1037	1392	381
2000	1089	1103	1542	394
2001	1093	1107	1565	396

Table 4.1: Price indices and their development.

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Battery limit investment

The battery limit investment denotes all investments necessary to have all required equipment for process operations installed on-site. This includes structures necessary to house the process as well as delivery and installation of all individual assets. One major part of these cost will the the process equipment. As the exact manufacturers and models of the equipment will not be known in early design stages, an approach similar to the one in sec. 4.1.1 still needs to be employed. In contrast to before now the cost for individual pieces of process equipment will be considered separately. Each piece of equipment will have an specific feature that most influences its cost. For vessels and reactors this might be volume, while for heat exchangers the required heat exchange area is essential. The price for an piece of equipment i C_E^i can again be approximated by a simple power law

$$C_E^i = C_B^i \left(\frac{Q_E^i}{Q_B^i} \right)^{M^i} . \tag{4.3}$$

A reference price C_B^i is multiplied by the determining quantity Q^i normalized to a reference state Q_B^i and raised to the power M^i specific to each piece of equipment. Reference prices and quantities for various installations can be obtained from literature.

add reference

If information on the process conditions are available, they also can be considered in price calculations. Aside from the mere size of the equipment the process conditions will also have an affect on the expected cost. The predominant factors to that respect are pressure, temperature and the question wether corrosive or reactive media, which will require more resistant materials, will be present. Furthermore if a more detailed choice of process equipment is known this is considered as well. For example an plate-fin heat exchanger might be more expensive than a tubular model with the same heat-exchange area. In order to account for all those effect a form factor f_F is applied to the equipment cost

$$C_E^i = C_B^i \left(\frac{Q_E^i}{Q_B^i} \right)^{M^i} f_F^i = C_B^i \left(\frac{Q_E^i}{Q_B^i} \right)^{M^i} \underbrace{\left(1 + f_C^i + f_M^i + f_P^i + f_T^i\right)}_{=f_F^i} . \tag{4.4}$$

Where f_F denotes the form factor, f_C corrects for design complexity, f_M for material selection, f_P adjusts for extreme pressures and f_T for temperature.

As in the previous section all reference prices need to be corrected to compensate for the temporal price development, Here again the already discussed indices are used. Furthermore can regional changes in price structures be considered. Here again have correction factors to prices in an reference region in the world (e.g. USA) been published.

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In addition to the purchased cost, the costs for installing the process equipment have an significant effect on the total needed investment of the process. These installation costs include:

- Installations costs
- Piping ,valves and electrical wiring
- Control system
- Structures and foundations
- Insulation and fire proofing
- Labour fees

Those again can be expressed as correction factors to the equipment price. Depending on the status of the information available they can be expressed as one unified factor or broken down to each specific category. One however needs to bare in mind, that costs for piping and valves – pieces of equipment in direct contact with process media – will be affected by the process conditions in a similar way as the actual equipment, whereas the other categories are more likely to remain unchanged. Thus attention needs to be paid, in with fashion the factors will be applied.

A word should be said to the cost for the control system. Most obtainable data will most likely refer to a decentralized control system, as it has been in use for many years. WIth ever more powerful computers a centralized approach, namely model predictive control (MPC) is becoming more relevant. As the structure for such a control system may vary significantly from the common designs, the cost factors may as well.

Services

The utility investments and off-site investments are often referred to as services. Therein included are all measures necessary to supply the process with the media required for operations. This includes but is not limited to generation and distribution of energy, steam, process gases. The utility investments in this context refer to all investments within the greater production site but out of the battery limits of the process. Off-site investments contain everything not contained in the site such as roads, power cables, communication systems or waste disposal. All these costs are expressed as fractions of the equipment cost at moderate temperature and pressure. This means, when applying these fractions, the factors f_M, f_P and f_T should not be considered at this point.

Once again in early design stages one has to resort to factors derived for statistical data, to calculate the cost of raw materials, energy and support media such as lubricants, heat or catalysts. If more detailed information on process streams is available the approach should be refined.

The cost of raw materials C_{RM} can then be calculated if the streams of individual raw materials m_i as well as their specific cost are known.

$$C_{RM} = \left(\sum_{i}^{N_{RM}} \dot{m}_i \cdot C_{RM}^{i} \right) \cdot t_{op}. \tag{4.5}$$

Much in the same way the cost for energy can be calculated. This is once more done for each individual pice of equipment, rather then for the whole process as it has been done for the raw materials. Hence with the needed energy for equipment i with respect to energy carrier j e_{ij} along with the price for energy carrier j C_{EC}^{j} the total energy cost C_{EC} can be assessed.

$$C_{EC} = \left(\sum_{i}^{N_E} \sum_{j}^{N_{EC}} \dot{e}_{ij} \cdot C_{EC}^{i} \right) \cdot t_{op}. \tag{4.6}$$

Working capital

The working capital includes all investments necessary for process operations. This means raw materials, payroll, extended credit to customers and so on. In contrast to all other costs the working capital can partially be retrieved when the process stops operations. How different types of cash flows, extended or owed credit should be handled will be disused in sec. 4.2. This section will focus on how raw materials and process media contribute to the total process cost.

Total investment

When all contributions to the total investment are considered an estimate for the total price of the process can be calculated

$$C_P = \sum_{i}^{N_E} \left[C_B^i \left(\frac{Q^i}{Q_B^i} \right)^{M^i} \left(f_F \cdot f_{PIPE} + \sum_j f_j \right) \right] + C_{RM} + C_{EC} + C_{FILL} \tag{4.7}$$

It should be emphasized that in early design stages these calculations will at best yield an order of magnitude estimate for the expected cost of implementing a chemical process. Most literature sources give an accuracy of $\pm 30\%$ [3]. As the poject progresses more and more information becomes available an a more accurate estimate can be prepared. Those often rely on actual proposals from prospective manufacturers and suppliers.

4.2 Investment criteria

The total cost of a project its a very important measure to decide wether to undergo a certain endeavor. However in a complex financial system it cannot be taken as the sole factor to compare investment

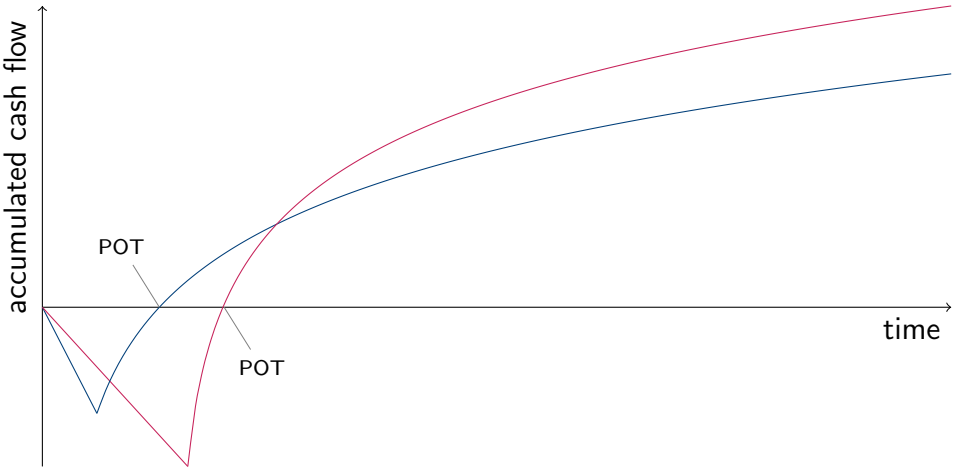

Figure 4.1: Accumulated cash flows over project life cycle.

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alternatives. Different other indices are used to measure the attractiveness of an investment. One main destination can be made between different measurements. This is wether the time value of many is considered. First two measurements – payback time and return of investment (ROI) – not considering time value will be discussed. By analyzing time dependent cash flows indices can be derived, that yield a more realistic view of the economic situation. Out of those the net present value (NPV) as well as the discounted cash flow rate of return (DCFRR) are introduced.

4.2.1 Single period estimation methods

Specific production cost

Payback time

Payback time is the time necessary to earn the total investment of the process. It is also often referred to as the break even point. A profitable venture will form that point on begin to make money. A shorter payback time is a measure for an more attractive investment.

$$POT = \frac{\text{capital expenditure}}{\text{incoming cash flow / period}} \tag{4.8}$$

Return of investment

The return of investment is defined as

$$ROI = \frac{\text{average return / period}}{\text{capital expenditure}} \cdot 100\%. \tag{4.9}$$

In terms of capital expenditure (CAPEX) a congruent measure for all compared options needs to be chosen.

CAPEX als total investment oder Buchwert oder ...

4.2.2 Multi period estimation methods

Net present value

Discounted cash flow rate of return

5 Uncertainty in process modeling

6 Cryogenic air separation

6.1 Process model

6.1.1 Distillation columns

6.1.2 Heat exchanger

6.1.3 Compressors

6.1.4 Turbine

6.2 Process Economics

7 Conclusion and further research

Todo list

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