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Fabrieksvoorontwerp
Vakgroep Chemische Procestechnologie

Onderwerp

Normal- and iso-butyraldehyde production from proylene and synthesis gas using a water soluble rhodium catalyst

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Keywords

Normal-butyraldehyde, iso-butyraldehyde, oxo-process, water soluble rhodium catalyst, hydroformylation.

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Summary

The main objective of this FVO is to design a profitable normal-butyraldehyde plant, with a capacity of the butyraldehyde production plant is set on 100,000 t/a of n-butyraldehyde. Other objectives for this design are to maximize normal-butyraldehyde yield on the raw materials, minimize heat loss, wastes and emissions. The plant is designed for an annual onstream period of 48 weeks. The remaining 4 weeks are utilized for equipment maintenance. The economic lifetime of the plant is assumed to be 15 years. Product specifications for normal-butyraldehyde is 98.5 % w/w purity, the specifications for the by-product iso-butyraldehyde is 99.5 % w/w purity. Water content may not exceed 0.3 % w/w.

Butyraldehyde is produced from carbon monoxide, hydrogen and propylene. The synthesis gas composition is H_2:CO = 1.1:1. The propylene feed is 95 % pure, the 5% impurity consists entirely of propane. The conversion of propylene to butyraldehyde in the reactor is 89 %, a major sideproduct from the reactor is propane, formed in a reaction of propylene and hydrogen. The conversion of propylene to propane is 4%. The catalyst is rhodium with as a ligand the Na-salt of TPPTS (triphenylphosphate-trisulfonate), which form a water-soluble complex. In this way the catalyst is immobilized in the water phase. The reactor is A CSTR, it operates at 120 °C, 50 bar. Propane is purged as an inert, the resulting gas mixture is sold as fuel gas. Feed streams are propylene, 20 °C, 25 bar, and syngas, 20 °C, 30 bar.

The product specifications have been met, the normal butyraldehyde produced is 99.8 % w/w pure, water content is zero. The byproduct iso-butyraldehyde is 99.46 % w/w pure. This corresponds to a 89.7 % conversion of the propylene feed to butyraldehyde, carbonmonoxide conversion is 89.7 %, hydrogen conversion is 85.6 %. The feed losses in the product streams are neglected. The production target for normal-butyraldehyde, 100,000 T/a, is achieved, the production capacity is 101,000 T/a. Iso-butyraldehyde production is minimized by proper catalyst choice. The iso-butyraldehyde production capacity is 6,001 T/a. The total fuel gas stream leaving the plant is 1,740 T/a. Low pressure steam is generated, it leaves the process at 127 °C, 2.5 bar, and at 111 °C, 1.5 bar.

The design is roughly based on an oxo process by Hoechst Chemie in Germany.

The economic analysis of the design gives for the total investments I_T according to Taylor 87.3 M$, Miller gives 73.3 M$ and Zevnik-Buchanon gives 77.9 M$. The Pay Out Time POT for Taylor, Miller and Zevnik-Buchanon respectively are 1.5, 1.3 and 1.4 years. For the Return On Investment ROI is calculated that Taylor gives 39 %, Miller gives 52 % and Zevnik-Buchanon 47 %. Their respective Internal Rates of Return IRR are 27.5 %, 43.6 % and 39.0 %.

\+ Continuous / batch plant / semi batch
* What is your final investment estimate? } uncertainty range
POT
IRR

* Wast ratios kg/kg product?

* Location demands

Acknowledgements

We would like to express our sincere thanks to professor De Graauw, for providing us with this highly challenging assignment. The FVO offered us an opportunity to use the knowledgethat has been handed to us over these years in an integrated assignment.

Much appreciated thanks to Ir. Luteijn for supplying us with some relevant documentation and guidance.

Our gratitude also extends to Jan Smit, for providing us with a room, where we could make coffee.

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Appendices

Gerard.

Ron + Ewt.

1. Introduction

The design for the butyraldehyde-production described in this report is made in the course of the 'FabrieksVoorOntwerp' (FVO), which is dutch for preliminary plant design. The FVO has an important place in the education for chemical engineers at the University of Technology in Delft.

The two isomeric butyraldehydes, normal- and isobutyraldehyde, C_4H_8O occur naturally in trace amounts in tea leaves, certain oils and tobacco smoke. But commercially the two butyraldehydes are produced almost exclusively by the oxo-reaction.

The total 1988 worldwide volumes of n- and i-butyraldehyde were $4.4*10^6$ T/a and $7.7*10^5$ T/a respectively. For this design the n-butyraldehyde production is assumed to be 100,000 T/a. This is equal to about 2.3% of the worldmarket. The n-butyraldehyde should be 98.5 wt% pure and the iso-butyraldehyde should be 99.5% pure. These specification are the quality specifications, obtained from Union Carbide[19].

Both n- and i-butyraldehyde are important intermediates for the chemical industry. The production of n-butanol and 2-ethylhexanol use 90% of all the n-butyraldehyde world production; 2-ethylhexanol is most widely used as the di(2-ethylhexyl) phthalate ester for the plasticization of flexible PVC.
The remaining 10% of the worldwide n-butyraldehyde production is used in the production of polyvinylbutyral, 2-ethylhexanal, trimethylolpropane, methyl amyl ketone, and butyric acid.
About 70% of the worldwide isobutyraldehyde production is utilized for the production of isobutyl alcohol and isobutyraldehyde condensation and esterfication products. The other isobutyraldehyde derivative markets are neopentylglycol (for water-borne and alkyd-surface coatings), isobutylacetate (solvent for nitrocellulose coatings) and isobutylidene diurea (slow release fertiliser).

The earliest modification of the oxo-proces employed cobalt hydrocarbonyl as a catalyst. This catalyst gave a higher n : iso ratio of 3:1. In the mid-1970s a process employing a rhodium catalyst ($HhCO[P(C_6H_5)_3]_3$ was commercialized by Union Carbide. The advantages of a rhodium-based catalyst are a lower temperature, lower pressure and a higher n/iso ratio of 10:1. In the mid-1980s Ruhrchemie (now Hoechst) used a technology based on a water soluble rhodium catalyzed process. A n/iso ratio of 16 : 1 is obtained. The design presented below demonstrates a process using such a water soluble rhodium catalyst. This design is limited to the production of butyraldehyde.
The production of 2-ethylhexanol or another product will not be considered.

* product outlets V

* annual worldwide prod. capacity V

* technologies o.k. V

2. Basic Hypothesis

2.1 Plant capacity

The capacity of the butyraldehyde production plant is set on 100,000 T/a of n-butyraldehyde. Other objectives for this design are to maximize normal-butyraldehyde yield on the raw materials, minimize heat loss, wastes and emissions. The plant is designed for an annual onstream period of 48 weeks. The remaining 4 weeks are utilized for equipment maintenance. The economic lifetime of the plant is assumed to be 15 years.

2.2 Battery limits

The battery limits are the raw chemicals needed for the process, propylene and synthesis gas, as they are supplied by other producers, and off-gas streams which represent value because of their composition, and two product streams. The battery limits for the process are represented in figure1.

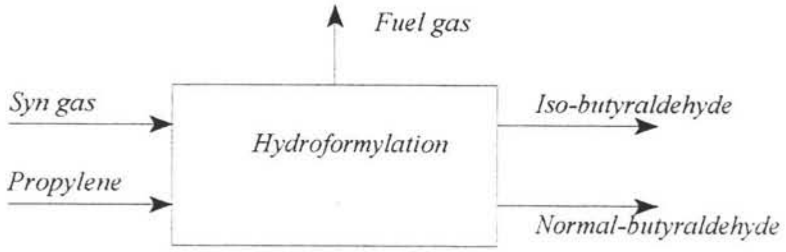


Figure 1: *Black box diagram for the process*

The stream specifications for the battery limits are given below in table 1.

Table 1: *Battery limits for the butyraldehyde plant*

Stream name	Number	Mass flow (kg/s)	Temperature (°C)	Pressure (bar)	Phase
Syn gas feed	2	6322	20	30	*gas*
Propylene feed	3	8815	20	25	*liquid*
Fuel gas	41	1952	36	19.5	*gas*
Iso-butyraldehyde	43	746	36	3.8	*liquid*
Normal butyraldehyde	39	12482	35	4	*liquid*

2.3 Process route

The process route chosen is a classical oxo-process. The production of butyraldehyde is based on the reaction of propylene with synthesis gas:

$$2\ CH_3\text{-}CH{=}CH_2 + 2\ CO + 2\ H_2 \rightarrow OCH\text{-}CH_2\text{-}CH_2\text{-}CH_3 + CH_3\text{-}CH(CO)\text{-}CH_3 \qquad \textbf{(1)}$$

An important side reaction is the formation of propane from propylene and hydrogen:

$$CH_3\text{-}CH{=}CH_2 + H_2 \rightarrow CH_3\text{-}CH_2\text{-}CH_3 \qquad \textbf{(2)}$$

Both reactions are exothermic:
$\Delta H_{r,1}$ = -261.6 kJ/mol C_4H_8O
$\Delta H_{r,2}$ = -84.7 kJ/mol C_3H_8

The reaction mechanism for the hydroformylation is

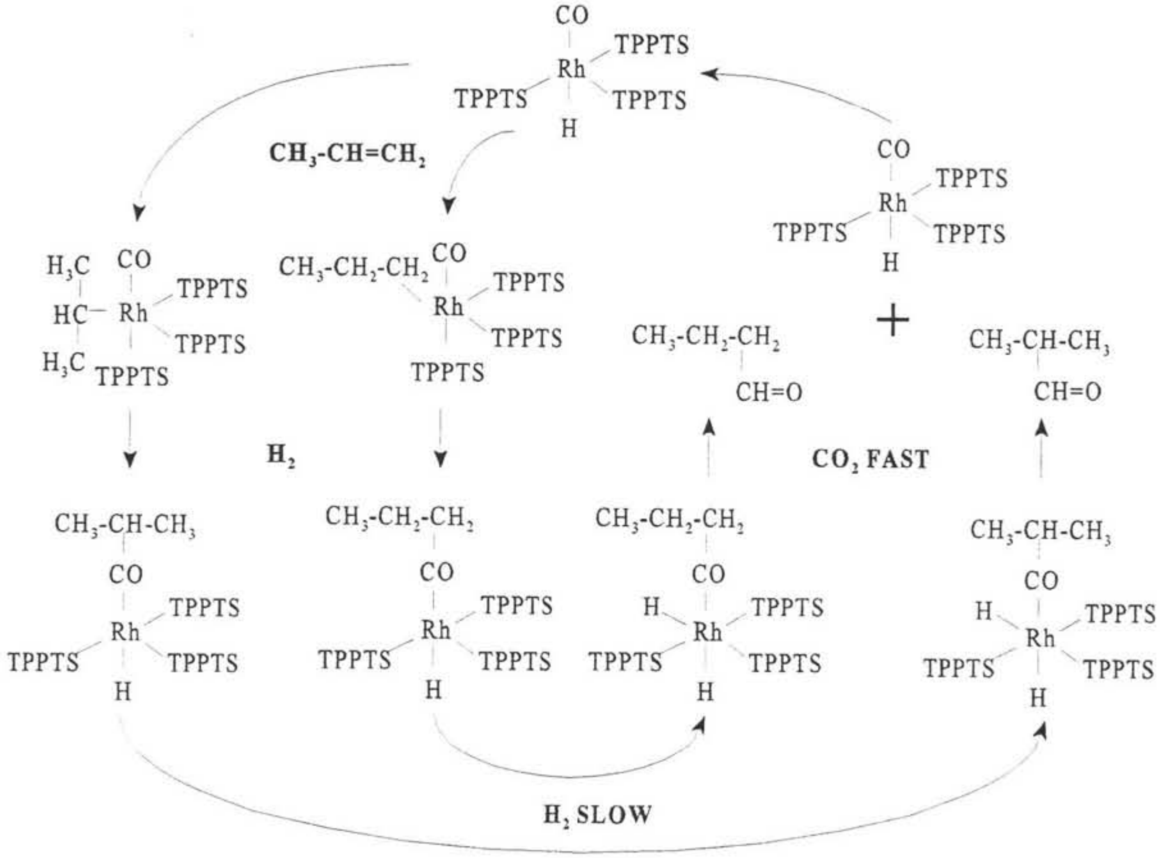


Figure 2: *Reaction mechanism of the hydroformylation reaction*

Is hier niet op zijn plaats.

The main advantage of the process described below in comparison to a classical oxo proces is the use of a rhodium catalyst, with the ligand TPPTS, which provides higher selectivity and reaction rates at milder conditions than the cobalt catalyst which is used in classical homogeneous oxo processes. The process is described in the following blockscheme.

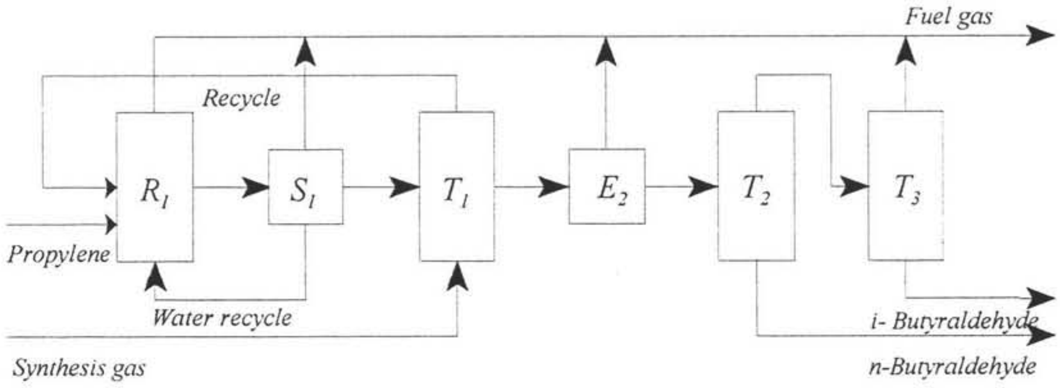


Figure 3: *Block scheme of the oxo process*

Where R_1 is the hydroformylation reactor, S_1 is the settler, T_1 is the stripper, E_2 is an expander, T_2 is the distilliation column where n-butyraldehyde is separated from the lighter components, *i.e.* i-butyraldehyde, water and propane, propylene etc. In T_3 the iso product is separated from the lights and water.

2.4 Additional specifications

2.4.1 Feed

Typically a chemical grade propylene is used. It is 95 % pure and the impurity in the proylene feed is assumed to consist of 5 mass % of propane. Synthesis gas consisting of H_2 and CO in a molar ration of 1.1:1 is utilized as a process feed. Inerts entering the plant through the synthesis gas feed are purged along with the propane from the propylene feed, and the propane that is formed in the reactor. They merely influence the value of the fuel gas leaving the process. They are not taken into account.

2.4.2 Products

Commercial n-butyraldehyde is 98.5 % pure on a molar basis. It should not contain more than 0.3 % water (w/w). Iso-butyraldehyde must meet the same specifications concerning water content, but overall purity required is 99.5 % on a molar basis. Quality specifications are obtained from Union Carbide Corp[19].

2.4.3 Utilities

The main utility required is water, both for cooling and for reactor water supply, as for generating steam. Furthermore 380 V 3 phase and 10 kV electrical current is required. Superheated or pressurized steam has to be supplied to cover reboiler duties of both distillation columns.

2.4.4 Location

The plant is located in the Botlek area. Raw materials needed for the process are easily supplied, and due to a high concentration of chemical industries a good infrastructure is present for shipping and transport by railway or truck. Also safety measures are at a high level, well educated personnel and staff is available. Another main advantage of locating the plant among other chemical industries is that product can immediately be sold. This eliminates the need for extensive storage facilities. The same goes for synthesis gas and propylene supply.

2.5 List of compounds

All compounds in the process are listed in table 2, along with their primary physical properties, some toxicity data and the world market price used in the economy calculations[16]. Furthermore the Chemical Abstract (CAS) numbers are listed.

Table 2: *List of compounds in the process*

Name	CAS no.	Formula	RMM (g/mol)	BP[1] (°C)	MP (°C)	ρ[2] (kg/m3)	MAC value (ppm)	Hazard rating	Lethal[3] dose	Price[4] ($/ton)
Propylene	115-07-1	C_3H_6	42	-47.7	-185.2	519	-	3	>1000[a]	270
Propane	74-98-6	C_3H_8	44	-42.0	-187.0	500	1000	3	>1000[a]	150
n-Butyraldehyde	123-72-8	C_4H_8O	72	74.8	-99.0	830	200	3	10[a]	678
i-Butyraldehyde	78-84-2	C_4H_8O	72	64.5	-65.9	789	200	3	100[a]	703
Water	7732-18-5	H_2O	18	100.0	0.0	997	-	1	>1000[a]	4.25
Carbon monoxide	630-08-0	CO	28	-191.5	-205.0	1.2	25	3	1.2[a]	21.8[a]
Hydrogen	1333-74-0	H_2	2	-253.0	-259.3	0.088	-	3	-	21.8[a]
Rhodium	7440-16-6	Rh	103	1966	3727	2410	-	3	-	73.13[7]
Sulfuric acid	7664-93-9	H_2SO_4	98	290	10.5	997[6]	1(8)	3	2140[c]	-(8)
TPPTS	-	$P(m\text{-}C_6H_4SO_3\text{-}Na)_3$	568	-	-	-	-	-	>5000[c]	-
Toluene	108-88-3	C_7H_8	92	110.4	-94.5	866	100	3	5000[c]	-
Sodium Hydroxide	1310-73-2	NaOH	40	1390[5]	318.4	997[6]	-	3	500[c]	-
Triisodecylamine	25376-45-8	$C_{10}H_{14}N$	148	99	280	778	-	3	-	-

ligand

[1] All boiling points given at atmospheric pressure

[2] Densities given at 20 °C and atmospheric pressure

[3a] LD_{50} and LD_{100} in ppm

[3b] Given as mg/kg

[4a] Syngas price is given as c/m^3

5) Properties given for solid NaOH

6) Water density; solution density is dependent on the solute concentration

(7) $/g

(8) Given as mg/m^3

[9] Regeneration costs are lumped in general utilities

3. Process structure and flowsheet

3.1 Process structure

The process structure will be explained using the Process Flow Sheet (PFS), which is given in appendix 1A. Appendix 1B represents a zoom in on the reactor section for a detailed layout of the process control. The PFS is drawn using the technical drawing package, AutoCAD 12. The flowsheet is simulated with the chemical flowsheeting package, ChemCAD 3.20. The mass and heat balances are represented in Appendix 3.

The PFS is roughly based upon the patent by Hoechst[2]. The original flowsheet by Hoechst has been modified to meet the objectives mentioned in the Basic Hypothesis. The changes concern the heat management and the water recycle. Because of minimal losses of butyraldehyde in expander E2 no washing column was required. The distillation section had to be designed separately. This was done according tot the heuristic rules given in Stephanopoulos [12].

The PFS will be discussed in four sections *i.e.* the main stream (red), the fuel gas streams (green), the water recycle (marine blue) and the water/steam streams (turquoise).

●The main stream.
Syngas feedstream 2 is compressed in compressor C2 and fed to stripper T1, where it used as a stripping agent to remove unreacted propylene from product stream 19. After being compressed by compressor C1 syngas stream 7 is led to the reactors R1a, R1b and R1c.
Propylene feedstream 3 is pumped to a slightly higher pressure than the pressure of the reactorsection by pump P2. This is required to compensate for pressure drops caused by heat exchangers H3 and H1, which preheat the propylene stream resp. 24 and 20 before it is fed to the reactorsection.
Water and fresh ligands, stream 1, are added to the water recycle to compensate for water losses and ligand degeneration.
settler S1
Stream 14, leaving the reactorsection, is split by expander E1 into water recycle stream 21, fuel gas stream 13 and product stream 19. Stream 19 is stripped in stripper T1 by stream 25 as described above. Product stream 26 is cooled in heat exchangers H3 and H4 before entering expander E2. The volatile compounds (fuel gas), released by the pressure drop, are separated from product stream 28 and are mixed with fuel gas streams 17 and 29. Product stream 31 is mixed with stream 18 from exapnder E1 in vessel V1. The newly formed product stream 33 is preheated in heat exchangers H11 and H10. The preheated stream 36 is pumped into distillation column T2 by pump P3. In distillation column T2 the product stream 34 is split into the raw i-butyraldehyde stream 35 and the pure n-butyraldehyde stream 38, which is cooled in heat exchanger H7. Stream 35 is led into distillation column T3 to be separated from its lights to give the pure i-butyraldehyde stream 43, which is cooled by heat exchanger H11.

●The fuel gas streams.
Fuel gas stream 8, leaving the reactor section is mixed with fuel gas stream 13 from settler S1 and enters expander E1 as stream 12. In expander E1 stream 12 is partially condensed to recover butyraldehydes. Fuel gas stream 17 leaving expander E1 is mixed with fuel gas stream 30 leaving expander E2 and fuel gas stream 29 from distillation column T3 top form fuel gas stream 32. Stream 32 is cooled in heat exchanger H10.

●The water recycle.
The water recycle, which contains the catalyst, leaving settler S1, stream 21, is cooled in heat exchangers H1 and H2. Stream 16 is mixed with the water and fresh ligands feed stream 1 and pumped into the reactor section by pump P1.

●The water/steam streams.
Water stream 4 is preheated in heat exchanger H4 and vapourized in heat exchanger H2.
Water stream 5 is vapourized in heat exchanger H7.

3.2 Thermodynamics

As a general thermodynamical model in the flowsheeting package Unifac was chosen. This model can be applied to enarly ideal gasses, the activity coefficients are calcualted from group contributions. This is a sound method when a large range of polar and non-polar groups are present in the process compounds. Enthalpies were calculated using a latent heat model. Exceptions to the overall K-value model are:

Reactor R1:	Predictive Soave-Redlich-Kwong (PSRK) was used for K-values, water-hydrocarbon immiscibility was selected. This model is effective for hydrocarbons at moderate to high pressures and temperatures.
Settler S1:	PSRK.
Stripper T1:	Grayson-Streed (GS) was used for modelling the stripper. It is a suitable model for simulating hydrocarbon reformer systems.
Distillation column T2:	PSRK.

For all equipement in the process, water-hydrocarbon immiscibility was selected.

4. Equipment design

4.1 Estimation of the kinetics of the hydroformylation reaction

Several tests on the activity of the rhodium catalyst under different reaction conditions have been done by Hoechst[2]. At a temperature of 125°C and a pressure of 50 bar the activity of the catalyst is 2.5 mol aldehyde/(g-atom Rh · min). This means that the activity of the catalyst $A \approx 11*10^3$ mol aldehyde/(mol cat · h). The conversion of propyleneto butyraldehyde is 89 %, the selectivity towards normal-butyraldehyde is 96 %, selectivity towards iso-butyraldehyde is 4 %. The side reaction of propylene and hydrgen towards propane is a gas phase reaction. Conversion of propylene to propane is 4 %.

In the literature[2] is stated that for a ligand:rhodium ratio of 50:1 any rhodium concentration in the range of 10-2000 ppm can be utilized. For a reasonable reactor volume, combined with the demands that solubility limits are avoided, a catalyst concentration of 200 ppm is chosen. The throughput of the reactor is 183278 mol of aldehyde per hour. This means that a total of 17.0 mol of rhodium is needed (1.75 kg). At a concentration of 200 ppm≡ $2*10^{-4}$ M, this gives a volume for the waterphase of $V = 85\ m^3$. Accounting for extra headroom for the gas phase, and taking into consideration a 70 % working volume, the total reactor volume $V_R = 120\ m^3$. This volume is used as a design value for the reactor.

4.2 Reactor design

Available reactor types

The two main reactor types that appear to be available for conducting a three phase liquid-liquid-vapour reactor, where one phase, the water phase, has a much larger volume than the other two phases, are a continuously stirred tank reactor (CSTR) and a bubble column. Vigourous mixing is required in the reactor, to ensure that the contact between the waterphase and the gasphase is adequate to achieve maximum conversion at minimal volume. A design will be made for both reactor types. A choice for a CSTR or a bubble column will be made on the basis of both designs.

4.2.1 Bubble column design

Overall design considerations

A bubble column has two main advantages over a CSTR, first of all its straightforward technology, and the abscence of a mechanical stirrer. A bubble column usually has no complicated internals, which ensures a low sensitivity to fouling, and a highly reliable and stable way of operation and design.

The primary conideration in designing the reactor should be that the full potential of the catalyst is utilized. The residence time of the gas in the water phase should be sufficient to achieve maximum conversion, but not longer. The reaction at the catalyst is therefore the rate determining step, mass tranfer and mixing in both phases must have shorter characteristic process times.Liquid-gas contacting is dependent on the flow regime in the bubble column. Designing the column therefore starts with determining the superficial gas velocity which gives the desired flow regime. For flow in the liquid phase, a CSTR model will be assumed. For the gas phase, a plug flow model, combined with axial dispersion is valid.

The cross-section of the column is determined by the mean superficial gas velocity,, which is defined as the volumetric gas flow rate at reactor temperature and pressure, divided by the vessel cross-section. The superficial gas velocity determines the flow regime in the reactor.

Flow and flooding

Flow phenomena in a three phase system such as the water-oganic-gas system under consideration are complicated due to a number of causes. The main cause is the large scale mixing to provide sufficient contacting surface of the liquid phase and the gas phase. The situation where the gas dominates the flow pattern is called flooding. This means that bypassing of the gas through the liquid phase occurs, without sufficient contacting.

There are two main causes for flooding:

-The column diameter is "too small", *i.e.* the gas rises as bubbles that occupy the total column diameter. This causes a flow pattern which can be compared to "slagging" in a fluidised bed.

-Rise velocity of the bubbles through the liquid phase is not high enough to provide ample shear stresses that break up the bubbles into smaller ones. Bigger bubbles have less contacting surface per unit of volume. This occurs at low superficial gas velocities, where the bubbles travel through the liquid phase at their free rising velocity

When the system is out of the flooding region, three different flow regimes can be present, dependent on the superficial gas velocity:

-Homogeneous flow is defined as the regime in which liquid circulatory flows are absent. All bubbles rise upward and mixing is only provided by the liquid in the bubble wake. This regime occurs at low superficial gas velocities ($<1\text{-}4\ \text{cm} \cdot \text{s}^{-1}$).

-The regime dominated by circulatory flows is called heterogeneous flow. Circulatory flows originate from local density differences at the bottom of the vessel due to uneven gas distribution over the sparger holes. The circulating liquid drags the gas bubbles through the vessel, providing higher shear rates, smaller bubble sizes and thus better mixing. Heterogeneous flow occurs at superficial gas velocities in the range of $4\text{-}80\ \text{cm} \cdot \text{s}^{-1}$.

-At superficial gas velocities above $1\ \text{m} \cdot \text{s}^{-1}$, the gas blows the liquid out of the column. This flow regime is called entrained flow. It should be avoided at all times.

The flow regime that provides adequate mixing and ample safety margin in the operating range is heterogeneous flow. Gas-liquid contact is intense, gas residence times can be manipulated to achieve full conversion.

Gas hold-up

The volumetric gas hold-up in bubble columns with a heterogeneous flow regime is given by

$$\epsilon = 0.6\,(v_{gs}^{c})^{0.7} \tag{1}$$

This means that for v_{gs}^{c} the gas hold-up is only 12 %. If the estimate of the rise velocity v_b is used this gives a hold-up of 23 %.

Bubble column design calculations

Since the water phase should be ideally mixed in comparison to the gas phase, the liquid mixing time t_m should be smaller than the gas residence time. The gas residence time is given by

$$\tau_g = \frac{V_w}{\phi_g} = \frac{H_w}{v_{gs}^{c}} \tag{2}$$

whereV_w is the liquid phase volume, ϕ_g is the volumetric gas flow, H_w is the liquid phase height and v_{gs}^{c} is the pressure corrected superficial gas velocity. Liquid mixing in the heterogeneous flow regime is described by a mixing time t_m. In general the mixing time is derived from the circulatory flow regime in the waterphase. When the volumetric circulatory flow is divided by the tank volume, a circulation time t_c is obtained. As a rule

$$t_m = 4t_c \tag{3}$$

The mixing time of the waterphase is given by

$$t_m = 4t_c = 11(g v_{gs}^c T_v^{-2})^{-0.33} \frac{H_w}{T_v} \tag{4}$$

where T_v is the column diameter. Mixing in the gas phase is given by a dispersion coefficient D_{eg}

$$D_{eg} = 78(v_{gs}^c T_v)^{1.5} \tag{5}$$

The dispersion coefficient varies and thus the backmixing is strongly dependent on the column diameter T_v. For small column diameters the gas flow through the column will have a strong plug flow character. As T_v increases backmixing will increase, and thus the gas residence time will increase. D_{eg} is normally in the range of 10-100 $m^2 \cdot s^{-1}$. The design value of the dispersion coefficient is chosen to be 10. This will give the safest possible design. The column volume V_t is given by

$$V_t = \frac{\pi}{4} T_v^2 H_v \tag{6}$$

The gas residence time should be equal to or larger than the water phase mixing time. Van 't Riet and Tramper[3] give for the equilibrium bubble size d_b=6 mm. This bubble size is achieved by breaking up and terminal rise velocity for d_b = 6 mm for the heterogeneous flow regime is approximately 0.25 $m \cdot s^{-1}$. In the figure below, the mixing time t_m and the gas residence time τ_g are displayed as a function of the mean superficial gas velocity v_{gs}^c. All values are of t_m and τ_g are given at minimum H_v/T_v ratio (H_v/T_v>2), the design value of the bubble column is 40 m^3.

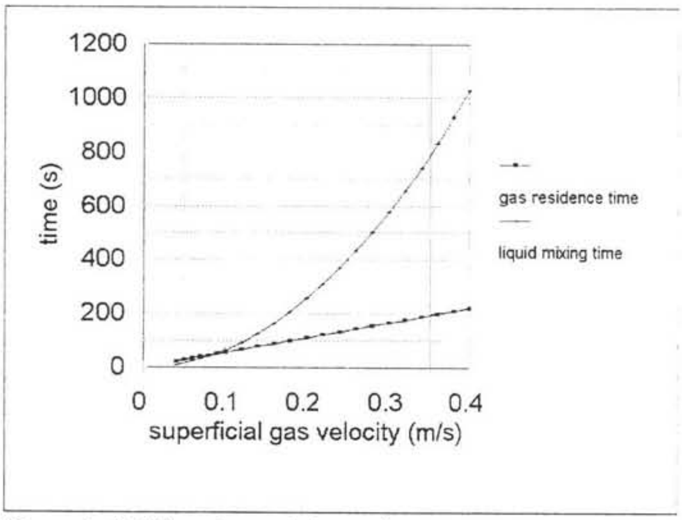


Figure 4: *Bubble column mixing regime*

As is obvious from figure 4 the mixing time t_m is only smaller than the residence time τ_g in the range of very small superficial gas velocities (0.04- 0.08 $m \cdot s^{-1}$). In this region the heterogeneous flow regime is not yet fully developed. The flow is unstable, leading to more gas bypassing and larger coalescense rates. From this figure must be concluded that for the given flow rates and dimensions, no proper bubble column design can be made in the heterogeneous flow regime. For this reason further design calculations are not usefull.

4.2.2 CSTR design

Introduction

A CSTR provides adequate gas dispersion, to ensure maximum contacting surface between the gas phase and the water phase. In the 1970s, it was usual to specify radial-flow, flat-blade turbines. Since then, however, several new impeller designs have become available[4]. A good dispersion can be achieved by using a multiple impeller system, existing of a combination of radial-flow impellers mounted below axial-flow, high effiency impellers. The preferred gas-sparger arrangement is a ring-sparger mounted below the lowest impeller with a diameter between 0.5 and 0.75 times the diameter of the impeller.

Flooding and dispersion

Flooding is a main problem to be avoided. The gas rises directly through the impeller to the liquid surface. An increase in impeller speed at fixed gas flow leads to a situation where the impeller disperses the gas radially. This situation is referred to as "loading" when the gas reaches the vessel wall, but does not recirculate below the impeller. If the impeller speed is increased further, the gas eventually recirculates throughout the whole of the tank volume. The impeller speed at which this complete dispersion occurs is called N_{cd} (cd stands for complete dispersion). Increasing the impeller speed beyond this point does not change the overall flow pattern in the tank. The increase in agitation intensity, however, leads to an increase in gas holdup and mass-transfer rate. In the turbulent regime, the gassed flow pattern depends primarily on two dimensionless variables, the aeration number N_A and the Froude number Fr.
N_A is defined as:

$$N_A = \frac{gas\ flowrate}{pumping\ capacity\ impeller} = \frac{\phi_g}{ND^3} \tag{7}$$

where ϕ_g = Gas flow rate [m^3/s]
N = Impeller rotation speed [s^{-1}]
D = Impeller diameter [m]

The Froude number is defined as:

$$Fr = \frac{inertial\ forces}{gravitational\ forces} = \frac{N^2 D}{g} \tag{8}$$

Warmoeskerken and Smith[5] stated that the maximum aeration number at which flooding occurs can be calculated by:

$$N_{A,FL} = C_{FL} Fr (\frac{D}{T})^{3.5} \tag{9}$$

where C_{FL} = Constant (flat-blade turbine C_{FL}=30; concaved-blade turbine C_{FL}=70)
T = Tank diameter [m]

An increase in viscosity slightly decreases the gas-handling ability of the flat-blade impeller, but has little effect on the transition to flooding with the concave-blade impeller. This is another advantage of the concave-blade impeller.

The aeration number for the transition to a flow pattern where the gas is completely dispersed is given in equation 10:

$$N_{A,CD} = C_{CD}\left(\frac{D}{T}\right)^{0.5} Fr^{0.5} \tag{10}$$

where C_{CD} = Constant (flat-blade $C_{CD} = 0.2$; concaved-blade $C_{CD} = 0.4$)

The minimum Froude-number that must be exceeded if the turbine is to retain any cavities (behind the blades) needed to achieve an adequate gas dispersion is equal to 0.045. With equation 7 to 10 the following flow regime can be drawn for the concave blade:

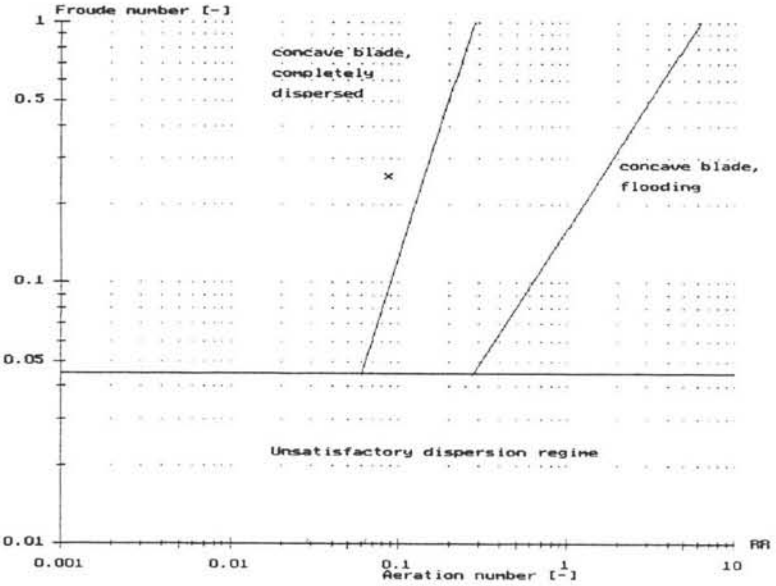


Figure 5: *CSTR flow regime as a function of aeration number*

The height H of the tank is equal to two times the diameter of the tank, T. There are three reactors present, each has a volume of 40 m^3. This gives: T = 2.9 m.
The stirrer diameter D = T/3 = 1.0 m.

The stirrer speed N is chosen to be 100 rpm. These values give the Froude number Fr = 0.28, well above the minimum value of 0.045. The gas flow is calculated as stated below:
Total gasflow in the reactor is 184.71 mol/s (propylene+hydrogen+carbon monoxide). ChemPROP is a computer program which calculates pure compound and mixture properties on the basis of thermodynamical data. With ChemPROP the molar density is calculated to be 1580 mol/m^3. So the gasflow Q_g in the reactor is: 184.71 / 1580 = 0.117 m^3 / s. The aeration number becomes :

N_A $= 0.117 / (1.67*1.0^3) = 0.07$

The values for Fr and N_A are drawn in figure ~~6~~ 5 (the point marked with x). This point shows that the reactor is completely dispersed.

Power requirements

The power drawn by an impeller strongly correlates with the cavity formation process and the associated gas flow pattern. With an increase in cavity size, the power draw of the impeller decreases.

Table 3: *Power numbers for different impeller types (Re > 10.000)*

Effect of impeller type on Power Number	
Impeller Type	Power Number (Po)
flat blade disc turbine	5.50
concave blade turbine	3.20
high efficiency impeller	0.32

Several assumptions are made:
-In each reactor two stirrers are installed
-The stirrer speed N is 100 rpm (1,66 rotation per second), taken from the article of Deshpande & R.V. Chaudhard[6].
-stirrer diameter D = 1.0 m

With these assumptions the following calculation can be made:
The Reynolds-number Re is calculated with equation 11:

$$Re = \frac{\rho N D^2}{\eta} = 7.32 \times 10^6 \tag{11}$$

where: ρ = density water = 1000 kg / m^3
N = stirrerspeed = 1.67 Hz
D = stirrerdiameter = 1.0 m
η = viscosity (120°C en 50 bar) =0.228*10^{-3} Pa.s

From table 3 is read that this Reynoldsgetal gives a Power-number Po equal to 3.2.

The Power number Po is equal to:

$$Po = \frac{P}{\rho N^3 D^5} = 3.2 \tag{12}$$

where P = added stirrer power
So the total added stirrer power is $P = Po\ \rho\ N^3 D^5 = 14.9*10^3$ Watt = $53.64*10^9$ J/h

The power is usually calculated in kWh. One kWh is equal to 1000*3600 = 3.6 MJ.
So the stirrer needs:53.64 MJ /3.6 MJ = 14.9 kWh per hour.

Rate determining step analysis

The mixing time for stirred vessels is given by Van 't Riet and Tramper[3]. They stated for the mixing time t_m:

$$t_m = \frac{6}{N}\,\frac{(T_v/D)^3}{Po^{0.33}} \tag{13}$$

All the variables are known, the mixing time has a value of:

$$t_m = \frac{6}{1.67} * \frac{(2.9/1)^3}{3.20^{0.33}} = 59.7\mathrm{sec} \tag{14}$$

In order to optimize the use of the catalyst in the waterphase, the mixing time should be smaller than the gas residence time. The gas residence time τ_g is determined by:

$$\tau_g = \frac{V}{\phi_g} = \frac{40}{0.117} = 341 \ \mathrm{sec} \tag{15}$$

Gas Holdup

Gas holdup is an important design parameter. Not only does it have a direct influenc on the mass-transfer rate, but an increased holdup may raise the liquid level or decrease the amount of liquid a tank can hold. The gas holdup is defined as:

$$\epsilon = \frac{V_g}{V_g + V_l} \tag{16}$$

Gas holdup is a function of the physical properties of the liquid, the impeller system, the power input and the gas rate. It can be predicted by the following correlation:

$$\epsilon = C_\epsilon \left(\frac{P_g}{V_l}\right)^A v_{sg}^B \tag{17}$$

J. Smith and K. J. Myers[7] have found that the following constants can be used:
$C_\epsilon = 0.18$
$A = 0.33$
$B = 0.67$

In correlation 18 the gas flowrate is expressed in terms of the superficial gas velocity, v_{sg},

$$v_{sg} = \frac{\phi_g}{\frac{\pi}{4} T^2} = \frac{0.117}{\frac{\pi}{4}(2.9)^2} = 1.77 cm/s \tag{18}$$

The total liquid volume needed is 85 m^3. In each tank the liquid volume $V_l = 28.33$ m^3.
This gives for the gas holdup:

$$\epsilon \ = \ 0.18*(14.9*10^3/28.33)^{0.33}\,(0.0177)^{0.67} = 0.095$$

So 9.5% of the total reaction volume is gasphase and 90.5% is liquid phase.

Sparger design

Spargers for high volumetric flow rates and low pressure drop should answer to the following conditions:

- -They should be as short as possible.
- -The shape of the sparger should be simple.

All extra length due to poor routing of the gas through the sparger will lead to an increased pressure drop, and thus an uneven distribution of the gas over the cross-sectional area of the reactor. For this reason, and for economic reasons (a sparger is sensitive to fouling at low gas flow rates) a circle-shaped sparger is mosty commonly used. Due to the considerations mentioned above, and to provide appropriate liquid residence times, most commercial bubble column reactors operate in the heterogeneous flow regime. For completely turbulent gas flow in the sparger ($Re_g > 2000$) the sparger design equation is:

$$\Delta P = 4f\frac{L}{D}\frac{1}{2}\rho_g v_g \qquad \textbf{(19)}$$

The maximum pressure drop over the sparger ΔP gives the desired sparger diameter D, since the sparger length L is equal to one third of the CSTR circumference πT. The minimum Re_g where the gas flow is completely turbulent is used to calculate the gas velocity v_g. Standard hole spacing in a sparger is 2-3 times the bubble diameter d_b. If the bubble diameter is considered to be 6 mm, the sparger holes are taken 15 mm apart.

Sizing of the CSTR

The dimensions of the CSTR are taken from the article, written by R.V. Roman and R.Z. Tudose[4]. They stated that adequate dispersion and transfer can be obtained in a CSTR that is proprortioned as in figure 6:

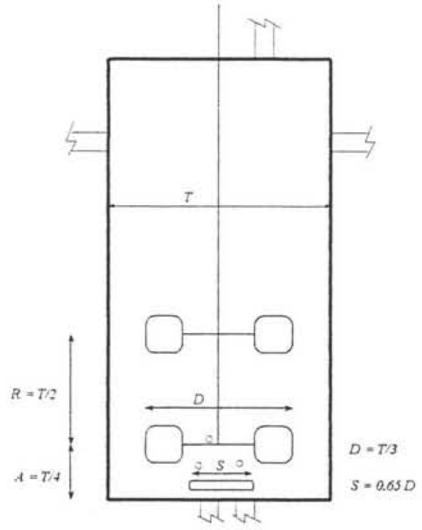


Figure 6: *Reactor sizing*

This gives for the dimensions of the CSTR:
T = 2.9 m
A = 0.73 m
H = 6.1 m
D = 0.97 m
S = 0.63 m
The reactor section thus consists of three vessels of 6.1 m high, and 2.9 m in diameter.

4.2.3 Conclusion

The most important conclusion that can be made when the two reactor designs are compared is that the CSTR provides the desired gas dispersion, and the bubble column does not. Therefore the CSTR is the most logical choice for the reactor. The main drawback of a CSTR, is that an axis for the stirrer has to be led through the reactor wall. The pressure difference over the seal is 49 bar. This is a represents a major safety problem.

4.3 Catalyst regeneration process

Process considerations

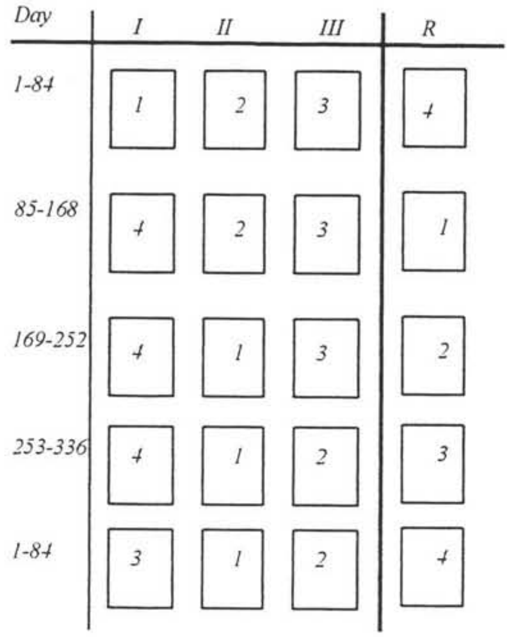
The most valuable part of the catalyst are the ligands. The main goal of regenerating the catalyst is to recover as much of the ligands as possible. The catalyst is poisoned by nickel and iron from piping and equipment. When the catalyst contains 20mg/l Fe and 0.7 mg/l Ni, it is at the end of its active lifetime. Regeneration means that these metals are removed. The water phase is acidified with aqueous H_2SO_4. By the acidification the ligands are made soluble in an organic phase. They are extracted in a solution of tri-isodecylamine in toluene. This organic phase is further extracted with dilute caustic to recover the TPPTS. About 93 % of the original TPPTS and rhodium complexes are recovered in the aqueous phase. It is replenished with fresh ligands and catalyst precursor in the form of rhodium acetate complexes.

Process description

Aqueous sulfonic acid (10% w/w)[1] is used on a 50 % w/w basis to acidify the spent catalyst solution. They are extracted with 20 % w/w tri-isodecylamine in toluene. The extracted catalyst solution is neatralize1d with 10 % w/w NaOH as they are recovered again in the aqueous phase. Regeneration takes place at 45 °C and atmospheric pressure. If the assumption is made that the organic phase has a density of approximately 800 kg/m^3, and equal volumes are used of each phase, the regenerator has approximately twice the volume of a reactor, 81 m^3. The volume of catalyst solution to be regenerated is 85/3 = 28.3 m^3. The liquid volume in the regenerator is 56.6 m^3, the reactor volume is 56.6/0.7 = 81 m^3. The same vessel is used for all regeneration steps. The regenerator is a stirred tank reactor. It is constructed of glass lined stainless steel, due to the pH cycles it is subjected to.
If however a continuous process is to be designed for the regeneration, three extra pieces of equipement are needed. After the acidification reactor, an extraction vessel is needed, followed by a settler-decanter. The organic phase containing the ligands then continues through a mixer, where the dilute caustic solution is added. Last step in the regeneration would be a mixer-settler, to separate the regenerated catalyst solution from the organic extractant, and to add fresh ligands. Because of the extra investment needed, and because of added process complexity, a bath configuration is chosen for the catalyst regeneration design.
A number of utilities are needed: A liquid turbine, to convert energy stored in the reactor contents at 50 bar can be regained as electrcity. This electrcity can be used to drive the stirrer for the regeneration process. A buffer vessel has to be installed between the reactor section and the regenerator, to avoid contact between a spent catalyst batch and a regenerated one. Due to limited information on the regeration process however no extensive design is possible.

Catalyst regeneration cycle

During the 336 days per year all reactors are on stream. If a particular catalyst batch is regenerated, the reactor is filled with fresh catalyst coming from the regenerator. To ensure fully continuous operation three reactors are needed.
The regenerative cycle is illustrated in the figure below. The reactors have roman figures, the regenerator is calles R, the different catalyst batches are numbered 1 to 4. The figure shows the position of the catalyst batches in approximately 80 day intervals. The first interval is day 1 to day 84, the second is day 84 to 168, etc etc.



Day	I	II	III	R
1-84	1	2	3	4
85-168	4	2	3	1
169-252	4	1	3	2
253-336	4	1	2	3
1-84	3	1	2	4

Figure 7: *Catalyst regeneration cycle*

4.4 Column Design

The process contains two standard (one feed, two outputs) distillation columns; the N/I-separation column and the I/light ends-separation column.The sizing of the column comprises mass flow rates and physical properties of phases at crucial points (cross sections) along the column. For distillation columns these points are always the top and the bottom of the column, and in the case of a pronounced pressure drop the top and bottom of the rectifying and stripping sections, respectively. The feed point conditions are then representative for the 'bottom' of the rectifying section and for the 'top' of the stripping section.

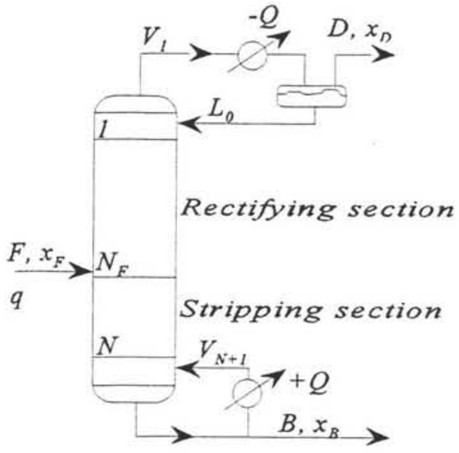


Figure 8: *Standard distillation column*

where F represents the feed stream, x_F is the feed liquid fraction, q is the feed quality, N_F is the feed tray, N is the bottom tray, 1 denotes the top tray, B is the bottom stream, x_B is the bottom liquid fraction, V_{N+1} is the reboiler vapour stream, L_0 is the liquid reflux, V_1 is the top vapour stream, D denotes the distillate flow, x_D is the distillate liquid fraction and Q denotes both reboiler and condensor duties.

4.4.1 Design equations

material and energy flows

The molar flow rate of vapour leaving the top of the column is:

$$V_1 = L_0 + D = D\,(R + 1) = V_{N+1} + F\,(1 - q) \tag{20}$$

The molar flow rate of liquid differs in the rectifying and stripping sections:

$$L_r = L_0 = D\,R \tag{21}$$

$$L_s = L_0 + q\,F = L_n = B + V_{N+1} \tag{22}$$

Thus, the molar flow rate of vapour entering the bottom of the column can be expressed as :

$$V_{N+1} = L_0 + q\,F - B = D\,R + q\,F - B \tag{23}$$

The operating reflux ratio is described as:

$$R = \frac{L_0}{D} \tag{24}$$

where q : thermodynamical conditions of feed
N : bottom tray/number of trays
N+1: gas inlet conditions
r : rectifying section
s : stripping section
o : liquid reflux conditions
index 1 denotes the top tray

For sizing purposes molar flows have to be transformed into mass flow rates. With molar flow rates and corresponding enthalpies the (heat transfer) duties of the condenser and the reboiler can be calculated, which are the basis for sizing condensers and reboilers.

$$Q_{con} = V_1 * H_{G,1} - L_0 * H_D = V_1 * H_{G,1} - D * H_D * (R + 1) \tag{25}$$

where H : molar enthalpy
indices G and D denote vapour and the distillate

In the case of partial condensation a two phase mixture leaves the condenser and after separation in the reflux accumulator (a flash drum) two distillates are produced which differ in phase state. The condenser duty in this case is:

$$Q_{con} = V_1 * H_{G,1} - \left(\frac{V_D}{V_1}\right) * V_1 * H_{G,D} - \left[1 - \left(\frac{V_D}{V_1}\right)\right] * V_1 * H_D - L_0 * H_D \tag{26}$$

where $H_{G,D}$: molar enthalpy of vapour product,
(V_D/V_1) : molar fraction of vapour in the two phase mixture leaving the condenser.

The reboiler duty is obtained from the overall energy balance:

$$Q_{reb} = Q_{con} + B * H_B + D * H_D - F * H_F \tag{27}$$

Indices B and F denote the bottom product and feed, respectively.

Tray column diameter.

The column diameter can easily be derived from the simple continuity relation for the vapour velocity:

$$u_G = \frac{(M_G/\rho_G)}{(\pi * D_{col}^2/4)} \tag{28}$$

where M_G : mass flow rate
ρ_g : density of the gas phase

Designing with an 80 % safety margin for the operating vapour velocity gives:

$$D_{col} = (4\ M_G/\pi * \rho_G * 0.8\ u_{G,\max})^{0.5} \tag{29}$$

The major limiting factor is the vapour velocity at which flooding occurs, which can be estimated from the well known Souders correlation:

$$u_{G,\max} = C_{tr} * [(\rho_L - \rho_G)/\rho_G]^{0.5} \tag{30}$$

where C_{tr} is the so-called capacity (gas load) coefficient, that can be described as:

$$\begin{aligned} C_{tr} = 0.0129 + 0.1674*T_s + (0.0063 - 0.2682*T_s)*F_{LG} \\ + (-0.008 + 0.1448*T_S)*F_{LG}^2 \end{aligned} \tag{31}$$

F_{LG} represents the liquid-vapour flow parameter:

$$F_{LG} = (\frac{M_L}{M_G})*(\frac{\rho_G}{\rho_L})^{0.5} \tag{32}$$

Tray column height

The total column height consists of the height between the top and bottom tray, the height above the top tray (needed for vapour disengagement and mist elimination) *(a)*, the height below the bottom tray (gas inlet and liquid discharge) *(b)*, and a skirt *(c)*. The total column height can be estimated from:

$$h_{col}\ (m) = h_{TB} + 1.5(a) + 2.5(b) + 2(c) \tag{33}$$

The height between top and bottom tray can be estimated from the number of actual trays and the tray spacing:

$$h_{TB}\ (m) = (N_{col} - 1)*T_s \tag{34}$$

where N_{COL} is the number of actual trays and is related to the overall column efficiency:

$$E_{col} = \frac{N}{N_{col}} \tag{35}$$

Packed column options

In packed columns the contact between gas and liquid phases is obtained on the surface provided by the packing.The function of packing is to promote fluid turbulence and mass transfer by dispersing the liquid, which, ideally, flows as a film over the surface of the packing. There are two type of packings: random and structured. These two types of packings require different design approaches. First the design procedure for random packings will be discussed.

Random packing: Raschig-rings.

The following values must be known:
Q_G, Q_L : volumetric gas and liquid flows
ρ_G, ρ_L : gas and liquid density
H_{col} : column height
d_p : nominal diameter of the packing
F_P : packing factor

These last two values can be derived from fig. 6.6[11], which is especially for Raschig-rings.

Next the value for φ must be calculated from:

$$\varphi = \frac{Q_L}{Q_G} * \sqrt{\frac{\rho_L}{\rho_G}} \tag{36}$$

Now from fig.6.7[11] the gas velocity, v_G, can be calculated from:

$$v_G * \sqrt{\frac{\rho_G * F_p}{\rho_L * g}} \tag{37}$$

Packed columns are usually designed at 70 % of their maximum load, so v_G will be replaced by $0.7 * v_G$. The cross-section and the diameter of the column are given by:

$$A_{col} = \frac{Q_G}{v_G} \tag{38}$$

$$d_{col} = \sqrt{\frac{4}{\pi} * A_{col}} \tag{39}$$

The volumetric liquid fraction ϵ in the column follows from:

$$v_L = \frac{Q_L}{A} \tag{40}$$

$$\epsilon = 1.2 * [\frac{v_L^2}{g * d_p}]^{\frac{1}{3}} \tag{41}$$

The 'dry' pressure drop can be calculated from:

$$\Delta p_d = 0.80 * \rho_G * v_G^2 * F_p * H_{col} \tag{42}$$

The 'wet' pressure drop can be calculated from:

$$\Delta p = \Delta p_d * (1 - 3.5\epsilon)^{-3} \tag{43}$$

Structured packing: MELLAPAK 250 Y

First of all the liquid-vapour flow parameter, F_{LG} must be determined:

$$F_{LG} = (\frac{M_L}{M_G})*(\frac{\rho_G}{\rho_L})^{0.5} \tag{44}$$

The values of C and $C_{G,\max}$ follow from fig. 6.39[11], which produces the capacity coëfficiënt:

$$C_{SP} = C \times C_{G,\max,Mellapak\ 250Y} \tag{45}$$

The corresponding maximum gas velocity is given by:

$$u_{G,\max} = C_{SP} \times [\frac{\rho_L - \rho_G}{\rho_G}]^{0.5} \tag{46}$$

which produces the gasloadfactor:

$$F_{sp} = 0.8*U_{G,\max}*(\rho_G)^{0.5} \tag{47}$$

In this equation the factor 0.8 indicates that the design point is placed at 80 % of the maximum capacity. The corresponding column diameter follows from:

$$D_{col}\ (m) = 1.1284*(\frac{M_G}{F_{sp}*\sqrt{\rho_G}}) \tag{48}$$

Determining the Murphree-efficiency according to the Maxwell-Stefan approach

The Murphree efficiency is given by

$$E_{MV} = 1 - \exp(-N_{oy}) \tag{49}$$

where the throughput number, N_{oy}, is represented by:

$$N_{oy} = \frac{k_{oy}*A}{Q_g} \tag{50}$$

where: A: phase interphase area at the tray = $0.90*A_{col}*A_{spec}$
A_{col} : cross-sectional area of the column
A_{spec}: specific interphase area

The throughput coefficient, k_{oy}, is given by:

$$\frac{1}{k_{oy}} = \frac{\beta}{k_{12}{}^{V}} + \frac{\alpha * m}{k_{12}{}^{L}} \tag{51}$$

where: $k_{12}{}^{V}$: throughput coefficient for the gasphase = D_G/δ_G
D_G : diffusion coefficient in the gasphase
δ_G : boundary layer thickness in de gasphase
$k_{12}{}^{L}$: throughput coefficient for the liquidphase = D_L/δ_L
D_L: diffusioncoefficient in the liquidphase
δ_L: boundary layer thickness in the liquidphase

From the following equations α and β can be calculated:

$$\alpha = 1 + x_1 * [\frac{\Delta H_1{}^{vap}}{\Delta H_2{}^{vap}} - 1] \tag{52}$$

$$\beta = 1 + y_1 * [\frac{\Delta H_1{}^{vap}}{\Delta H_2{}^{vap}} - 1] \tag{53}$$

where $\Delta H_1{}^{vap}$: heat of vapouration of n-butyraldehyde
$\Delta H_2{}^{vap}$: heat of vapouration of i-butyraldehyde
x_1: molfraction n-butyraldehyde in the liquid phase
y_1: molfraction n-butyraldehyde in the gas phase

The volumetric distribution coefficient is given by:

$$m = K * \frac{\rho_G}{\rho_L} * \frac{Mw_G}{Mw_L} \tag{54}$$

where ρ_L : density of the liquidphase
ρ_G :density of the gasphase
Mw_L: molar weight of the liquidphase
Mw_G: molar weight of the gasphase
K: distributioncoefficient

The column efficiency is given by

$$E_{col} = \ln[1 + E_{MV} * (s - 1)] / \ln(s) \tag{55}$$

where s: side dimension of a cross-section = 1.2

4.4.2 Results of the Column Calculations

For all three columns the internal diameter and the height of the column have been calculated. If the columns consisted of two sections, rectifying section (r.s) and stripping section (s.s), the diameter of each section was determined. All calculations have been carried out according to the theory described in the paragraphs above. The column calculations are represented in appendix 5A.

Table 4: *Internal diameter and height of the n/i-column*

N/I-column	Dint (r.s) [m]	Dint (s.s) [m]	Hcol [m]
sieve tray (ChemCAD)	1.83	2.13	49
sieve tray (calculated)	1.56	1.71	49
Raschig rings	2.67	2.91	49
MELLAPAK 250Y	1.19	1.25	49

Table 5: *Internal diameter and height of the I/lights column*

Iso/light ends-column	Dint (r.s) [m]	Dint (s.s) [m]	Hcol [m]
sieve tray (ChemCAD)	0.31	0.15	11
sieve tray (calculated)	0.24	0.13	11
Raschig rings	0.42	0.14	11
MELLAPAK 250Y	0.19	0.06	11

Table 6: *Internal diameter and height of the stripper*

Stripper	Dint (s.s) [m]	Hcol [m]
sieve tray (ChemCAD)	0.84	7
sieve tray (calculated)	0.69	7
Raschig rings	0.94	7
MELLAPAK 250Y	0.43	7

Determining the Murphree efficiency of the N/I-column gives for the column efficiency, E_{COL} 94.9 % when using sieve trays. Thus it is not useful to use any kind of packing to improve the column efficiency. The separation in the I/light ends is a simpler separation because of the fact that at about 70 °C the process becomes a gas-liquid separation. For this reason an even higher column efficiency is expected (so an assumed column efficiency of 75 % is more than reasonable). So the I/lights column is also equipped with sieve trays and no packing is applied. Because of the large gas flows that run through the stripper a packing is no option. A packing would cause great instabilities in the column.

4.5 Heat-exchanger/ vaporizer design

Design strategy

1 Define the duty (heat-transfer rate,flow-rates, temperatures)
2 Collect the physical properties.
3 Decide on the type of exchanger to be used.
4 Select a trial value for the overall coefficient U.
5 Calculate the mean temperature difference.
6 Calculate the required area.
7 Choose exchanger layout.
8 Calculate the individual coefficients.
9 Calculate the overall coefficients and compare with the trial value. If the calculated value differs significantly from the estimated value, substitute the calculated for the estimated value and return to step 6.
10 Calculate the pressure drop; if unsatisfactory return to steps 7 or 4 or 3 (in that order of preference).
11 Optimize the design (repeat steps 4 tot 10, as necessary, to determine the cheapest exchanger that will satisfy the duty).

4.5.1 Design equations

The general equation for heat-transfer across a surface is:

$$Q = UA\,\Delta T_m \tag{56}$$

where Q = heat transferred per unit time (W)
U = overall heat-transfer coefficient ($W/m^2{}^\circ C$)
A = heat-transfer area (m^2)
ΔT_m = mean temperature difference (°C)

• U

For heatexchange across a typical heat-exchanger tube the relationship between the overall coefficient and the individual coefficients is given by:

$$\frac{1}{U_0} = \frac{1}{h_s} + \frac{1}{h_{sd}} + \frac{d_o \ln (d_o/d_i)}{2\,K_w} + \frac{d_o}{d_i}\left(\frac{1}{h_s} + \frac{1}{h_{sd}}\right) \tag{57}$$

where U_0 = overall coefficient based on shell side surface of the tube ($W/m^2{}^\circ C$)
h_s = shell side coefficient ($w/m^2{}^\circ C$)
h_t = tube side coefficient ($w/m^2{}^\circ C$)
h_{sd} = shell side dirt coefficient ($w/m^2{}^\circ C$)
h_{td} = tube side dirt coefficient ($w/m^2{}^\circ C$)
k_w = thermal conductivity of the material ($w/m^\circ C$)
d_i = tube inside diameter (m)
d_0 = tube outside diameter (m)

•Shell side coefficient, h_{nb}.

The heat-transfer coefficient is dependent on the nature and conditions of the surface and it is not possible to present a universal correlation that will give accurate predictions for all systems.

The reduced pressure correlation given by Mostinski[8] (1963) is simple to use and gives values that are as reliable as those given by more complex equations.

$$h_{nb} = 0.104(P_c)^{0.69}(q)^{0.7}[1.8(\frac{P}{P_c})^{0.17}+4(\frac{P}{P_c})^{1.2}+10(\frac{P}{P_c})^{10}] \tag{58}$$

where P = operating pressure (bar),
P_c = liquid critical pressure (bar),
q = heat flux (W/m^2).

•Tube side coefficient, h_t.
An accurate estimate of the heat-transfer coefficient can be made by using the Eagle and Ferguson equation, developed especially for water:

$$h_i = 4200\ (\ 1.35\ +\ 0.02\ t)\ \frac{u_t^{.8}}{d_i^{.8}} \tag{59}$$

where h_t = tube side coefficient for water (w/m^2°C)
t = water temperature (°C)
u_t = water velocity (m/s)
d_i = tube inside diameter (m)

•Dirt coefficients.
A good estimate of these coefficients can be made with table 12.2[8], p 570. For the product stream in general the dirt coefficient for light hydrocarbons, 5000 W/m^2°C was used. The cooling medium is water, the dirt coefficient for cooling water is 3000 W/m^2°C

•Thermal conductivity.
The thermal conductivity of metal can be estimated with table 12.6[8], p 591. The thermal conductivity of stainless steel is 16 W/m°C.

- ΔT_m

The mean temperature difference is given by:

$$\Delta T_m=\Delta T_{lm}*F_t \tag{60}$$

where F_t = temperature correction factor
ΔT_{lm} = logarithmic mean temperature difference (°C)

•Correction factor, F_t.
The correction factor is a function of the shell and tube fluid temperatures and the number of tube and shell passes.

It is normally correlated as a function of two dimensionless temperature ratios:

$$R = (T_1 - T_2)/(t_1 - t_2) \tag{61}$$

$$S = (T_1 - T_2)/(t_2 - t_1) \tag{62}$$

where T_1 = inlet shell-side fluid temperature
T_2 = outlet shell-side fluid temperature
t_1 = inlet tube-side temperature
t_2 = outlet tube-side temperature

For a 1 shell:2 tube pass exchanger the correction factor is given by:

$$F_t = \frac{\sqrt{(R^2+1)}\ln(1-S)/(1-RS)]}{(R-1)\ln[\dfrac{2-S[R+1-\sqrt{R^2+1}]}{2-S[R+1+\sqrt{R^2+1}]}} \tag{63}$$

•Mean temperature difference, ΔT_{lm}.
For counter-current flow the logarithmic mean temperature is given by:

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln\dfrac{(T_1 - t_2)}{(T_2 - t_1)}} \tag{64}$$

- A

An estimate of A can be made, if Q and inlet and outlet temperatures are known, with a estimated U from table 12.1[8], p 570. For this heat-transfer area a new heat-transfer coefficient can be calculated. With this heat-transfer coefficient a new transfer area can be calculated. This has to be recalculated untill convergence is achieved.

- Shell and bundle diameters.

If the heat-transfer area is known or estimated the number of tubes can be calculated. An estimate of the bundle diameter D_b (in mm) can than be obtained from the equation:

$$D_b = d_o\left(\frac{N_t}{K_1}\right)^{1/n_1} \tag{65}$$

where N_t = number of tubes
d_0 = outside tube diameter (mm)
K_1, n_1 = empirical constants, for an 1 shell:2 tube passes resp. exchanger 0.249 and 2.207 (triangular pitch, p_t= 1.25 d_0).

The shell diameter is twice de bundle diameter.

- Tube side pressure drop

The tube side pressure drop (in Pa) can be obtained from the equation:

$$\Delta P_t = N_p \left[8 j_f \left(\frac{L}{d_i}\right) \left(\frac{\mu}{\mu_w}\right)^{-m} + 2.5\right] \frac{\rho u_t^2}{2} \qquad \textbf{(66)}$$

where N_p = number of tube passes
u_t = tube side velocity (m/s)
L = length of one tube (m)
d_i = Inside diameter (m)
ρ = density of the fluid (kg/m^3)
j_f = tube side friction factor (can be obtained from figure 12.24)[8]

- Shell side pressure drop.

A good estimate of the shell side pressure drop can be obtained from the following table 7.

Table 7: *Shell side pressure drops for different fluid viscosities*

Viscosity (Ns/m^2)	**Pressure drop (kN/m^2)**
<1	35
1-10	50-70

- Critical heat-flux.

The maximum critical heat-flux can be predicted with the Mostinski reduced pressure equation:

$$q_c = 3.67 \cdot 10^4 \, P_c \left(\frac{P}{P_c}\right)^{0.35} \left[1 - \left(\frac{P}{P_c}\right)\right]^{0.9} \qquad \textbf{(67)}$$

where q_c = maximum critical heat flux (W/m^2)
P = operating pressure (bar)
P_c = liquid critical pressure (bar)

- Maximum vapour velocity at liquid surface.

The freeboard between the liquid level and the shell should be at least 0.25 m. To avoid excessive entrainment the maximum vapour velocity at the liquid surface should be less than the velocity (m/s) given by the expression:

$$\hat{u}_{v,\max} = 0.2 \left[\frac{\rho_l - \rho_v}{\rho_v}\right]^{0.5} \qquad \textbf{(68)}$$

where ρ_L = liquid density (kg/m^3)
ρ_v = vapour density (kg/m^3)

4.5.2 Results

Because of the low process temperature, *i.e.* ca. 120 ° C, the ***minimum temperature difference*** for the heat-exchangers, normally ca. 15 °C, is chosen to be ca. 10 °C.
A full design of heat-exchanger H1 and estimations of the design of the other heat-exchangers is given in appendix

5B. The most important parameters in the design of a heat-exchanger are listed below.

Table 8: *Important design parameters of the heat-exchangers*

Equipment	Q (kW)	U (kW/m²°C)	$\Delta T_{ln,c}$ (°C)	A (m²)
H1	325	1.26	47.2	6
H2	6900	2.00	11.0	312
H3	192	0.30	30.8	21
H4	246	0.75	24.0	14
H5	5100	1.00	66.0	77
H6	6000	0.50	80.3	101
H7	1000	0.75	10.2	131
H8	5100	1.00	89.8	56
H9	76	2.00	28.9	2
H10	114	0.30	15.1	25
H11	38	0.30	26.5	5

The estimations of the heat-exchangers are based on a U-tube fixed head heat-exchanger, 16 mm external, 14 mm internal diameter tubes (4.8 m). The heat-transfer coefficient is estimated with the aid of table 12.1[8]. The logarithmic temperature difference is used (no temperature correction factor is applied). The tube side velocity (<2 m/s) is calculated to determine whether the estimated transfer area is realistic. H9 is operated with a cryogenic heat exchange fluid. The design of the heat-exchanger H1 is done with the strategy given in this chapter.

4.6 Pump design

Strategy

1 Define the duty (flow-rates, temperatures, pressure difference)
2 Collect the physical properties.
3 Decide on the type of pump to be used.
4 Calculate theoretical power.
5 Estimate/determine efficiencies and calculate the actual power.
6 Optimize design if unsatifactory (by repeating steps 3 to 6).

4.6.1 Design equations

- Theoretical power

The theoretical power can be obtained from the equation 69:

$$P_t = \frac{\Delta P \ Q_m}{\rho} = \Delta P \ Q_v \qquad \textbf{(69)}$$

where P_t = theoretical power (W)
ΔP = pressure differential across the pump (Pa)
Q_m = mass flow-rate (kg/s)
Q_v = volumetric flow-rate (m^3/s)
ρ = density of the fluid (kg/m^3)

- Efficiencies

The values given in figure 10.62[8], p 428, can be used to estimate the pump overall efficiency. Overall efficiency is chosen to be 75 %, which is a conservative estimate. Therefore the actual power is overdesigned.

- Actual power

Introducing the overall efficiency in the theoretical power equation the actual power is obtained:

$$P_a = \frac{\Delta P \ Q_m}{\eta_o} \tag{70}$$

where P_a = actual power (W)
ΔP = pressure differential across the pump (Pa)
Q_v = volumetric flow-rate (m^3/s)
η_o = overall efficiency (-)

4.6.2 Results

The calculation of the actual power can be found in appendix 5C . The results of these calculations are displayed in table 9 below.

Table 9: *Calculated theoretical and actual pump power*

Equipment	Theoretical power (kW)	Actual power (kW)	ChemCAD value (kW)
P1	16.76	22.35	22.37
P2	14.92	19.80	19.80
P3	0.46	0.61	0.60

The calulated powers conform to values obtained from the ChemCAD simulation calculations.

4.7 Reflux drum/gas-liquid separator design

Dimensions of a distillate reflux drum must be fixed to allow:
- droplet disengagement in the vapour phase
- enough surge time for the liquid phase

In the vapour phase droplet separation is achieved by limiting the vapour velocity according to Newton's law. Maximum vapour velovity is given by an empirical correlation:

$$v = K\sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \approx K\sqrt{\frac{\rho_L}{\rho_V}} \tag{71}$$

where v = vapour velocity (m/s)
K = velocity constant (m/s)

Both densities are given at design conditions. Typically K is 0.04 m/s for horizontal vessels having a wire mesh demister[10]. The value of the maximum allowable gas velocity is divided by 1.25, which gives a design value. If the value of v is known, the minimum free area for vapour passage can be determined. Normally surge time for reflux vessels to distillation columns are taken between 5 and 15 minutes. As a design value 10 minutes surge time is taken. Surge time is dependent on holdup time with the drum half full. The vessel diameter is calculated from:

$$d_{hsep} = 1.1284(\frac{M_G}{\rho_G}u_{hsep}\phi_G)^{0.5} \tag{72}$$

where ϕ_G is the fraction of the cross section which is occupied by gas. The length of the horizontal flash drum depends on the residence time and the fractional gas cross section,

$$L_{hsep} = \frac{V_L}{(1-\phi_G)\frac{\pi}{4}d_{hsep}^2} \tag{73}$$

Several cross sectional gas fractions are entered untill a liquid height to diameter ratio of approximately 0.5 to 0.6 is obtained.This gives a length to diameter ratio of around 5. Corresponding height of the liquid level follows from [11]:

$$h_L = d_{hsep}(0.9167 - 0.8333\phi_G) \tag{74}$$

Reflux drum calculation results

The conditions and throughputs for the reflux drums aregiven in table 10:

Table 10: *Conditions and throughputs for the reflux drums*

	GLS 1	GLS 2
Pressure (bar)	4	4
Temperature (°C)	104	15
Throughput L (kg/h)	37584	792
Throughput V (kg/h)	828	68
Vapour density (kg/m^3)	9.2	7.9
Liquid density (kg/m^3)	686	798
Vapour velocity v (m/s)	0.33	0.4

4.8 Compressor/Expander Design

In this process two compressors and two expanders are used, which perform polytropic compression or expansion. The required work for this compression/expansion can be calculated from:

$$-W = Z*\frac{R*T_{in}}{M}*\frac{n}{n-1}*[(\frac{P_2}{P_1})^{\frac{n-1}{n}} - 1] \tag{75}$$

where R : universal gasconstant, 8.314 J K^{-1}mol^{-1},
T_{in} : inlet temperature, K
M : molecular mass (weight) of gas,
Z: compressibility factor

The energy required to compress a gas, or the energy obtained from expansion, can be estimated by calculating the ideal work and applying a suitable efficiency value, in this case efficiency is taken to be 75 %.
The compressibilty factor, Z, is a function of the reduced temperature, T_R, and reduced pressure, P_R.
The polytropic exponent, n, is a function of X and Y, compressibility functions dependent on the reduced pressure, and m, the polytropic temperature exponent according to the following equation:

$$n = \frac{1}{Y - m*(1 + X)} \tag{76}$$

In this equation X = 0, Y =1 and for compression holds:

$$m = \frac{Z*R}{c_p}*(\frac{1}{E_p} + X) \tag{77}$$

and expansion can be described by:

$$m = \frac{Z*R}{c_p}*(E_p + X) \tag{78}$$

C_p is the average molar specific heat of the stream through the compressor/expander. The polytropic efficiency, E_p, is defined for compression:

$$E_p = \frac{polytropic\ work}{actual\ work\ required} \tag{79}$$

and in the case of expansion:

$$E_p = \frac{actual\ work\ obtained}{polytropic\ work} \tag{80}$$

The polytropic efficiency E_p is a function of the volumetric flow rate (m^3/s) and can be determined from fig 3.6 in Coulson and Richardson [8]. Entering the volumetric flow rate provides a value for m. Further substitution gives a value for n.

The polytropic work can calculated from equation (75). The actual work can be determined by dividing the calculated work by the efficiency of the compressor. The actual power of the compressor/expander is given by:

$$P = \Phi_m * W \tag{81}$$

where Φ_m is the mass flow rate.

Compressor and expander design values are given in table 11:

Table 11: *Compressor and expander design values*

Unit	W (kJ/mol)	W_{actual} (kJ/mol)	P (kW)
C1	-190	-292	47
C2	-1425	-2193	267
E1	1281	1971	-19
E2	3026	4655	-158

Compressor/expander design calculations are given in appendix 5D.

4.9 Settler design

The settler (unit S1) design is based upon two considerations. One is the availabilty of ample settling surface to achieve a good separation between the organic phase and the water phase. The other consideration is that the settler serves to separate the reactors from the rest of the process. Disturbances in the reactors will be reduced by the settler. The settler also serves as a 'storage' of cooling water, available for reactor control.

Drops of liquid settling with a velocity v_d will reach the phase boundary in

$$t = \frac{h}{v_d} \tag{82}$$

This time t should be smaller than the residence time τ.

$$\tau \leq \frac{l}{u} \tag{83}$$

where u is the horizontal liquid velocity. This velocity u is proportional to the volumetric throughput Q.

$$u = \frac{Q}{bh} \tag{84}$$

where b is the settler width. A good separation will be obtained when

$$\frac{v}{h} \cdot \frac{l}{u} \geq 1 \tag{85}$$

or in terms of the phase boundary A = bl

$$\frac{vA}{Q} \geq 1 \tag{86}$$

The volumetric throughput of the settler is 0.0407 m^3/s, the horizontal liquid velocity u is taken as 1 cm/s, settling velocity v_b is 0.5 cm/s, h = 0.2 l, b = 0.33 l. Settler dimensions are represented in the following table:

Table 12: *Settler dimensions*

l [m]	b [m]	h [m]	A [m^2]
11	3.7	2.2	41

4.10 Buffer Vessel design

The vessel V1 is installed to stabilize feed to the distillation columns T2 and T3. Surge time in the buffer vessel is chosen to be 15 minutes. The surge time τ_s is given by

$$\tau_s = \frac{V}{\phi_V} \tag{87}$$

where V is the volume of V1 and ϕ_V is the volumetric flow rate. The volumetric flow rate is 16.7 m^3/h. The vessel surge time is 15 minutes, so the volume of the vessel V1 is 4.2 m^3.

5. Process control

Process control equipment is installed to ensure safe and stable operation of the plant. A control system should be able to:

-Suppress the influence of external disturbances
-Ensure the stability of a chemical process
-Optimize the performance of a chemical process

5.1 Process control of the butyraldehyde plant; general considerations

Process conditions can be ensured to be within allowable limits by the application of controllers. In this plant seven types of controllers are used, which are pressure controllers (PC), temperature controllers (TC), flow controllers (FC), liquid level controllers (LC), ratio controllers (RC), composition controllers (CC) and speed controllers (SC). Flow in this chapter exclusively refers to volumetric flow rate.

Controllers having feedback configuration have been chosen instead of controllers having feedforward configuration. Feedforward controllers are not used, because of the following disadvantages:

-Requires identification of all possible disturbances and their direct measurement
-Cannot cope with unmeasured disturbances
-Sensitive to process parameter variations
-Requires good knowledge of the process model

A feedback controller operates by comparing process conditions to a given set point. If the process conditions do not meet the set point, control action is taken.

5.2 Process control of the different sections

Process control scheme design considerations are given for each plant section. The controller configuration is given in the process flow sheet, PFS, appendix 1.

The reaction section

The reaction section consists of the reactors R1a, R1b, R1c, the settler S1 and the stripper T1. These units cannot be controlled separately, because control action in this section is highly integrated.
Constant temperature and pressure in the reactor are essential to ensure the stability of the process. The pressure in the reactor is controlled by a pressure controller (PC) in the gas flows out of the reactors. The temperature in the reactor is controlled by a temperature controller (TC). The water-catalyst recycle stream 21 is cooled by the propylene stream 20 and a cooling water stream 23. The reactor temperature is coupled with a FC on the cooling water stream 23. If the reactor temperature increases the cooling water stream will increase as well. The recyclestream will enter the reactor at a lower temperature level.
A flowcontroller (FC) is installed in the propylene feed 3. The signal of the reactor temperature and the propylene flow enter a high switch selector (HSS). Here, limits are specified on the maximum reactor temperature and propylene flow. If the reactor conditions are within the operating range, the flow is to be maintained at its specified set point. If the temperature exceeds these limits, controller action will be taken by reducing the propylene flow. The formation of both butyraldehyde and propane, which are exothermic reactions, will be reduced.
The synthesis gas flow 2 is controlled by a ratio controller (RC). The ratio controller enables for the reactants to enter the reactor in the right stoichiometric ratio. If the propylene feed is reduced, the synthesis gas flow will be reduced as well. Both feed streams may not exceed an upper limit. A liquid level controller (LC) in the reactor enables for the right gas/liquid ratio in the reactor. Stirring is essential for good heat transfer and a good production rate. A stirring control device controls the stirring speed. If the stirrer fails, the reactor becomes a bubble column. In the bubble column the conversion becomes lower and heat tranfer becomes more difficult. In the worst case scenario the temperature in the reactor rises. To prevent any fire and/or explosion risks, the propylene and synthesis gas feed are closed. The stirrer controller is installed only for this worst case scenario.

The settler S1 serves as a buffer. This has the following advantages:

- Deviations in the reactor effluent will have less impact on the rest of the process.
- If the temperature in the reactor rises, cooling water can be obtained from the settler.

The percentage of butyraldehyde in the gas stream out of the settler should be minimized. A PC is installed in the outgoing gas stream 13 to ensure a constant pressure and low evaporation rate of butyraldehyde in the settler. The water catalyst recycle stream 21 is important for the reactor temperature control. A LC is installed in the water catalyst recycle stream to ensure a constant cooling recylce water flow. There is no need for a controller in the organic product stream 19. The outgoing product stream 19 is determined by the LC in stream 14, the LC in the water/catalyst stream 21 and the PC in gas flow 13.

The organic product stream 19 is led to stripper T1. The synthesis gas flow 25 to the stripper is controlled by the RC and the compressor control system. A too high pressure in the stripper is prevented by installing a pressure relief. If the pressure in the stripper exceeds the upper-limit, the valve opens until the pressure is at the setpoint. The outgoing product stream 26 is controlled by a RC on stream 26 and stream 19. If the settler stream 19 reduces, the outgoing stream 26 reduces also. The RC controls the holdup in the stripper.

The compressors C1 and C2

To prevent the discharge pressure of a compressor from exceeding an upper limit, a controller is installed. The installed PC is cascaded to the speed controller of the compressor engine. Usually a compressor is controlled by a PC and a FC [12]. Flow may not exceed an upper limit to keep the driver from overloading.
- By using pressure controllers on the reactors, settler and stripper the gas flow 11 from the stripper to compressor C1 does not exceed an upper limit. Compressor C1 has no need for a FC.
- The synthesis gas flow 2 has an upper limit and is controlled by a ratio controller. The capacity of compressor C2 is sufficient to handle this upper limit. A FC on the compressor C2 is therefore not necessary.

The expanders E1 and E2

Two expanders are installed in the butyraldehyde process:
- Expander E1 receives the gas stream leaving the reactor and the gas stream from the settler (stream 12). Pressure controllers are installed on those streams. There is no need for further control action. In the expander the incoming gas stream 12 will split up in a gas stream 17 and a liquid stream 18. Because the liquid stream 18 contains butyraldehyde, it is led to the distillation column T2.
- Expander E2 receives the product stream 26 from the stripper. This stream is controlled by a RC. There is no need for further control action. Stream 26 will also split up in a gas stream (stream 30) and a liquid stream with butyraldehyde (stream 31).

The Vessel V1

The liquid stream leaving the expander E2 (stream 31) is led to vessel V1. The liquid stream 31 is mixed with the liquid stream 18 from expander E1. The outgoing stream 33 is controlled by a FC. Because of the large residence time in the vessel, deviations in the streams 31 and 18 will be reduced. The FC ensures a constant flow to the N/I distillation column. A distillation column requires a constant feed for good operation.

The distillation columns T2 and T3

- The feed to the first distillation column T2 is controlled by the flow controller on stream 33 from the vessel V1. The bottom product of the first distillation column is n-butyraldehyde (stream 37).
Reboiler ratio control is recommended for the control of the bottom compositions [13]. A liquid level controller (LC) manipulates the liquid stream leaving as bottom product, and indirectly manipulates the reboiler vapour stream. The LC maintains a constant liquid level in the reboiler section. The heat input in the reboiler section is controlled by a FC

on the steam. In the topsection two other controllers are installed. A LC is placed in the condensor section. The LC controls the outgoing iso-butyraldehyde/light ends stream 35. A composition controller (CC) is mounted on the reflux stream. The CC is an infra-red spectroscope, which continuously measures the intensity of the C=O bound of normal and iso-butyraldehyde. If the intensity (proportional to concentration) of normal-butyraldehyde is too high, the reflux stream is increased. The n-butyraldehyde is led back to the distillation column. The n-butyraldehyde can now be recovered in the bottom section.

- The iso-butyraldehyde/light ends stream 35 is fed to the second distillation column T3. The light ends are the top product and iso-butyraldehyde is the bottom product. A high purity is required for iso-butyraldehyde. The bottom product is the most important stream in both T2 and T3. So both distillation columns have the same control system for the bottom section. The top sections are however slightly different. The top stream of distillation column T3 is a gas stream. A PC instead of a LC is installed in the topsection of column T3.

6. Process Safety

Safety is one of the most important aspects in designing and operating a chemical facility. Especially when the plant is located in the Botlek in the Netherlands, which is a densely populated area, an accident can have serious consequences for a large number of people. Another aspect of process safety is the protection of capital investment and operating costs. The production equipment and the design process itself, as well as the plant inventory, represent a significant value. In order for the proces to be profitable the off stream period of the plant has to be restricted to the design value. For process control and product specification garantee, the plant is provided with control equipment. In order to minimize all risks, a detailed analysis has to be made on the risks and hazards associated with operating the plant.

6.1 Properties of substances

The main property of substances that is responsible for the hazard it represents, is the flammability or its ability to form explosive mixtures with air, and the amount in which a compound is present. This is influenced by its boiling point under atmospheric conditions, and the state at which it is present in the process. Since the reactor is the unit that operates at the most severe conditions in the process, and the stripper has the highest inventory of flamable compounds, the physical state of the compounds and the explosion limits will be discussed for both units[14].

Reactor pressure is 50 bar, temperature is 120 °C. A large excess of water is present, free oxygen is absent, so the reactor is not in the flammability region of propylene. The same goes for propane and the other compounds listed below.
The stripper pressure is 45 bar, the temperature ranges from 75-115 °C. However, the stripper contains large amounts of flammable hydrocarbons and syn gas, and no water. It is not operated within the explosion region of the compounds in the process, but due to the composition of its inventory and the physical state of the inventory it represents a large risk. The exit stream is an overheated liquid, and will flash at atmospheric pressure. Safe operation of the stripper is essential. The only compound in the regeneration process which represents a serious flammability and explosion risk is toluene.

Table 13: *The lower (LEL) and upper explosion limits (UEL) and self ignition temperature for all the compounds*

Compound	LEL (vol %)	UEL (vol%)	Self ignition temperature (°C)
Butyraldehyde	1.8	9.5	375
Propylene	2.4	10.3	490
Propane	2.2	9.5	480
Hydrogen	4.0	75.0	400
Carbon monoxide	12.5	74.0	-
Toluene	1.3	7.0	535
Sulfuric acid	-	-	-
Isode cylamine	-	-	-
Sodium hydroxide	-	-	-
Rhodium	-	-	-

6.2 Toxicology of substances

The only acutely toxic compound in the process is carbon monoxide. It is present in relatively high concentrations and in large amounts. Its toxicity is emphasized by the fact that CO has by far the lowest MAC value (maximum allowable concentration), *i.e.* 25 ppm. [15]. Its LD_{100} = 1.2 mg/l. The MACs and LD_{50}s of the compounds in the process are given below.

Table 14: *Maximum allowable concentration (MAC-value) and lethal doses*

Compound	MAC (ppm)	LD_{50} (mg/l)
Carbon monoxide	25	1.2(1
Hydrogen	-	-
i-Butyraldehyde	200	10
n-Butyraldehye	200	100
Propylene	-	>1000
Propane	1000	>1000
Water	-	>1000
Toluene	100	5000
Sulfuric acid	1 mg/m^3	2140(2
Sodium hydroxide	-	40(2
Rhodium	-	-
Triisodecylamine	-	480(2

(1 LD_{100}
(2 mg/kg

6.3 Dow's Fire and Explosion Index

The Dow's Fire and Explosion Index (DFEI) gives an good insight into the fire and explosion risks of each process unit. The DFEI is based on two factors:

1. An Unit Hazard Factor (UHF), based on operational conditions and equipment used.
2. A Material Factor (MF), based on the flammability and reactivity of the compounds involved.

The product of the two factors gives the Fire and Explosion Index. Evaluation of the process indicates that the stripper has the highest fire and explosion risk. The stripper has a Fire and Explosion Index of 85.3. The unit with the second highest risk is the reactor with a DFEI of 76.2. The distillation column has a Fire and Explosion Index of 69.1. The reactor has a lower DFEI than the stripper, because of the great amount of water in the reactor. The water reduces the fire and explosion risk. The Dow's Fire and Explosion Index Classification Guide attributes a certain degree of hazard to a particular DFEI-interval:

Table 15: *Dow's Fire and Explosion Index-values and the Degree of Hazard*

DFEI	Degree of Hazard
1 - 60	Light
61 - 96	Moderate
97 - 127	Intermediate
128 - 158	Heavy
159 - up	Severe

As can be seen in table 15, the most dangerous process units have a moderate degree of hazard. The damage factor and the exposure radius can be calculated if the DFEI is known (Appendix 4). In table 16 the most important coefficients for the three most dangerous process units are given:

Table 16: *The UHF, MF, Damage Factor, DFEI and Exposure Radius for the three most dangerous process units*

	Stripper	N/I Distillation Column	Reactor
Unit Hazard Factor	3.95	2.89	7.67
Material Factor	21.60	23.9	9.93
Damage Factor	0.66	0.65	0.27
Fire and Explosion Index	85.32	69.07	85.32
Exposure Radius (m)	21.94	17.98	19.50

The Unit Hazard Factor is a measure of the propable relative damage exposure magnitude of the various combined contributing factors used in the Process Unit calculation (Appendix 4). This probable damage exposure magnitude is determined from figure 7 in The Dow's Fire and Explosion Index Hazard Classification Guide[21].
The Unit Hazard Factor is then identified as the Damage Factor and represents the overall effect of fire plus blast damage resulting from a fuel or reactive energy release caused by various contributing factors associated with the Process Unit.

The DFEI of a Process Unit produces an Exposure Radius which indicates those pieces of equipment that could be exposed to a fire or fuel-air explosion generated by the Process Unit being evaluated.

The conditions in the stripper T1 represent a 66% damage probability to 1512 m^2 of surrounding area and the conditions in the reactor represent a 27% damage probability to 1195 m^2 of surrounding area.

6.4 Safety features

In this section a number of important safety features are desribed. Process units such as the reactor and the stripper require these features for safe operation and protection of the plant and its surrounding from the hazardous contents and severe conditions in the process.

Essential safety features of the hydroformylation reactor

The huge mass of water keeps the reactor well out of the explosion region. Since no air or oxygen is used in the process, the main safety problem concerning the reactor is the fact that an exothermic reaction takes place. The reaction is carried out under pressure, a stirrer axis is led through the reactor roof.

1. To minimize leak rates from the stem seal, two conventional seals can be installed back to back[17]. This configuration is called a double mechanical seal. In the chamber between the seals, a high viscosity, high boiling oil is inserted and kept under higher pressure than the reactor itself. This way the oil keeps the reactor contents from leaking out along the stirrer axis. The oil is also a lubricating agent.
2. Detection equipment: The equipment must detect gaseous flammable hydrocarbons before their concentration reaches a certain level. Installation around pumps, compressors and the stirrer axis seal. Detectors for carbon monoxide and hydrogen are also obligatory.

Essential safety features of the stripper

The inventory of the stripper makes it a far more hazardous unit than the reactor. Therefore adequate safety features are installed.

1. Feed line emergency valves: The feed to the stripper must be cut as soon as a leak or a fire is detected.
2. Detection equipment: Hydrocarbon detectors, detectors for carbon monxide and hydrogen, all able to detect low concentrations. This equipment should control the valves closing the feed and exit lines of the stripper.
3. Smoke detectors: If a fire is accompanied by the development of smoke, smoke detectors can indirectly detect a fire.
4. Direct fire extinguishing medium feedline.

Miscellaneous safety features of the plant

1. Adequate water supply for fire protection.
2. Good access to the plant area and its surroundings for emergency vehicles and exits for personnel evacuation
3. Insulation of dangerously hot surfaces, such as the reactor wall.
4. Process control rooms should be isolated from the rest of the plant by a 1 hr fire wall, for plant shutdown in case of an emergency.
5. Snow and wind loads should be included in the design, to account for severe winter conditions.
6. Earthquake loads are neglected.
7. Snow removal and ice control equipment should be present on the plant site, roads should be kept clear of ice and snow at all times.
8. Communications, emergency telephones, a disaster response plan, including instructions for the surrounding population. Communications include radio, public address systems and safe location and continuous manning of the communications centre. The location of personnel on the plant site should be known at all times.

6.5 Hazard and operability analysis

A HAZard and OPerability (HAZOP) analysis is a systematic way of assessing the sensitivity of the process for a number of disturbances, and the hazards and risks that arise from these disturbances. The HAZOP also provides an indication on how to install proper process control equipment.

A HAZOP is done for the hydroformylation reactor, because it is the heart of the process, and for the stripper. The stripper is identified as the highest risk unit of the process by an analysis with the DOW's Fire & Explosion Index. The HAZOP for the reactor is presented below in table 17. The analysis of the stripper is represented in table 18.

Table 17: *Hazop of the hydroformylation reactor*

Guide Word	Deviation	Possible causes	Consequenses	Action Required
Not, No	No gas flow	1. No hydrocarbon or syngas available at Intermediate storage	Loss of feed to reaction section. Plant off stream	1. Ensure good communication with the supplier
		2. Failure of propylene pump and syngas compressor	As for (1)	2. Install backup pump and compressor 3. Carefull maintenance and checkups 4. Check compressor and pump design

Guide Word	Deviation	Possible causes	Consequenses	Action Required
		3. Line blockage, islolation valve is closed in error, liquid control valve (LCV) fails shut	As for (1), propylene pump overheats, recycle compressor overheats, transfer line subject to full pump/ compressor delivery	5. Covered by (3) 6. Install bypass for LCV 7. Patrol transfer line regularly
		4. Line fracture in feed and/ or recycle lines	As for (1), discharge of flammable gases to the atmosphere	8. Covered by (7)
	No water flow	5. Water feed pump failure	Reactor overheats, reaction runaway, catalyst degradation	9. Install flow controller (FC) on gas feed line 10. Install low level alarm 11. Install back-up water pump
		6. Water recycle line fracture	As for (5)	12. Covered by (9) and (10)
		7. Reactor exit line blockage	Pressure rise in reactor, runaway reaction, all gas goes through off-gas line, reactor overfills	13. Install high level alarm 14. Install vent on reactor off gas line
		8. Isolation valve fails shut	As for (7)	15. Covered by (13) and (14)
	No stirring	9. Stirrer engine failure	Gas bypasses the waterphase, no reaction	16. Checkups and maintenance, make sure that the engine has adequate power
		10. Stirrer breaks off	As for (9)	17. Ensure mechanical quality of stirrer, maintenance and checkups
More	More gas flow	11. Pressure drop in the reactor (suction)	Conversion drops, water is blown out of the reactor into off-gas line	16. Install entrance line FC
		12. More feed (compressor/ pump malfunction)	As for (11)	17. Covered by (16)
		13. More recycle	As for (11), propane concentration in the system goes up	18. Install FC on gas recycle line

Guide Word	Deviation	Possible causes	Consequenses	Action Required
	More water flow	14. More water feed	Reactor temperature drops, conversion drops, water load on system is raised	19. Install FC on water feed line
		15. More water recycle	As for (14), settling tank overfills	20. Install FC on water recycle line
	More P	16. Higher P gas feed	Reactor temperature goes up, leakage might occur, reaction is faster	21. Covered by (16)
		17. Lower conversion of gas feed	As for (16), conversion goes up as P goes up, selfregulating	
		18. Line blockage, due to fouling or valves failing shut	Reactor pressure rises, reaction is faster untill reactor pressure is equal to entrance line pressure, if the reactor P is higher than entrance line P, backflow may occur	22. Install one way valve in entrance line 23. Install high pressure alarm on reactor
	More T	19. More conversion	Reactor pressure goes up, more byproducts	24. Covered by (13) and (14)
		20 Higher T gas feed or recyle	Reaction is faster, reac-tor pressure goes up, loss of catalyst selectivity	25. Covered by (13), (14) and (20) 26. Monitor reactor temperature
		21. Higher T water feed or recycle	As for (20)	27. Covered by (25) and (26)
		22. Less water flow	As for (20)	28. Covered by (25), (26), (19) and (20)
Less	Less gas flow	23. Leaking valve or flange	Emissions of flammable hydrocarbons to atmosphere	29. Covered by (9), (16) and (18) 30. Regular inspection
		24. (1), (2), (3) and/or (4)	As for (1), as for (23)	31. Covered by (1)
	Less water flow	25. (24), (5), (6), (7) and /or (8)	As for (20)	32. Covered by (25) and (26)

Guide Word	Deviation	Possible causes	Consequenses	Action Required
	Less P	26. (2), (3) and/or (19)	Conversion drops, more feed to the reactor	33. Covered by (5) to (7)
	Less T	27. (24), (14), (15) and/or (17)	Loss of catalyst activity, accumulation of unconverted reactants in the system	34. Raise reactor temperature by reducing water recycle and feed
As well as	Products & byproducts	28. Loss of selectivity of the catalyst	Accumulation of byproducts in the system, off spec production	35. Fresh catatlyst feed, T control by recycle FC
		29. Wrong reaction conditions	As for (28), runaway might occur	36. Covered by (35), install water quench vessel
Part of	Only one product spec achieved, conversion not met	30. (28) and/or (29)	As for (28)	37. Covered by (35)
Other than	Other products	31. Wrong feed composition	Catalyst deactivation, runaway reaction, lower or higher T, P, off spec production	38. Monitoring of feed comp, also partly covered by (1)
		32. Wrong recycle composition	As for (31)	39. Monitoring, covered by (38) and (35)
	Maintenance, repairs	33. Equipment failure, flange leaks, stirrer failure, leakage along the axis of the stirrer, etc	Plant off stream	40. Monitoring, annual off stream period for repairs and maintenance

Table 18: *Hazop of the stripper*

Guide word	Deviation	Possible causes	Consequenses	Action required
Not, No	No syn gas flow	1. Syn gas compressor malfunction	Plant off stream, poor separation, no gas recycle	1. Install backup compressor 2. Maintenance, checkups

Guide word	Deviation	Possible causes	Consequenses	Action required
		2. No syn gas available at intermediate storage or supplier	As for (1)	3. Ensure adequate communication with storage managment and supplier
		3. Syn gas feed line blockage	As for (1)	4. Covered by (2)
		4. Valve fails shut	As for (1)	5. Covered by (2)
		5. Feed line fracture	As for (1), syn gas escapes to atmosphere	6. Covered by (2)
	No reactor effluent flow	6. Reactor exit line blockage	As for (1), all gas fed to the system escapes to off gas	7. Covered by (2)
		7. Liquid level in reactor too low	As for (6)	8. Install low level alarm
		8. Valve fails shut	As for (6)	9. Covered by (2)
		9. Reactor exit line fracture	As for (6), reactor effluent escapes to atmosphere	10. Covered by (2)
More	More syn gas flow	10. Syn gas compressor malfunction	Poor separation, liquid might be dragged into recycle	11. Covered by (1) and (2)
		11. More P at intermediate storage or supplier	As for (10)	12. Covered by (3)
	More reactor effluent flow	12. Higher water throughput	System cools down, poor separation	13. Install FC on reactor exit line
		13. Higher butyraldehyde production	Lower recycle, system heats up	14. Covered by (13)
	More P	14. More gas feed and recycle, higher reaction rates	Poor separation, system heats up	15. Install FC on reactor gas exit line 16. Increase water flow
		15. Higher reaction rates	As for (14)	17. Covered by (15) and (16)
	More T	16. More reaction	As for (14)	18. Covered by (16)

Guide word	Deviation	Possible causes	Consequenses	Action required
		17. Higher syn gas feed temperature	Better separation, system heats up	19. Covered by (16)
		18. Covered by (15)	As for (14)	20. Covered by (15) and (16)
Less	Less syn gas flow	19. Covered by (1) to (5)	As for (1)	21. Covered by (1) to (3)
	Less reactor effluent flow	20. Covered by (6) to (9)	As for (6)	22. Covered by (13)
	Less P	22. Covered by (6) to (9)	As for (6)	23. Covered by (1) to (3) and (8)
		23. Lower reaction rates due to catalyst deactivation	Higher recycle rates, poor separation	24. Add fresh catalyst to the reactor
	Less T	24. Covered by (23)	Poor separation	25. Reduce water flow
		25. Lower syn gas feed temperature	Poor separation, system cools down	26. Preheat syn gas by exchanging heat with reactor effluent

7. Process economics

7.1 Estimation of the production costs

Definition

"Cost, according to Webster, is the amount paid or given for anything ... hence whatever, as labor, self denial...,etc., requisite to secure a benefit."[18]

The total costs, K_T, can be estimated from:

$$K_T = K_A + K_F = K_A + K_O + K_P + K_I + K_L \qquad \textbf{(88)}$$

where K_A = general costs ($/a)
K_F = manufacturing costs ($/a)
K_O = indirect manufacturing costs ($/a)
K_P = production-volume dependent costs ($/a)
K_I = investment dependent costs ($/a)
K_L = semi-variable costs (labour costs etc.) ($/a)

This model is based on a classification of the total cost in two separate groups and four sub-groups. This is not the only classification possible. Different classifications, based on type of costs (labour, administration, raw material costs, etc.), the production-volume dependence etc., are also used.
The model is simplified by combining all costs, except for volume dependent costs, in the two sub-groups: production-volume and investment dependent costs. In such a case the K_A en K_O are included in K_I and K_L using a given distribution method , and the model becomes:

$$K_T = K_P + K'_I + K'_L \qquad \textbf{(89)}$$

The production-volume dependent costs, K'_P , are given by :

$$K'_P = a \cdot k_p \cdot P \qquad \textbf{(90)}$$

where P = the production capacity of the plant (kT/a)
k_p = costs of raw materials ($/kT)
a = correction factor for the production costs (which has not been taken into account).

k'_p can be calculated from:

$$k'_p = \sum_i^n v_i \cdot q_i \qquad \textbf{(91)}$$

where v_i = cost of raw material i ($/T)
q_i = amount of i needed for the production of 1 ton product (T/T)

The investments dependent costs can be estimated as a part of the investments.

$$K'_I = f \cdot I \tag{92}$$

where f = capital charge, fraction of the investments, determined by maintenance etc. (-)
I = total investments ($)

The semi-variable costs K'_L are often called the labour dependent cost, because they consist for a significant part of labour costs and can therefore be aproximated with:

$$K'_L = d \cdot L \tag{93}$$

where d = constant (varies with venture and product) (-)
L = total labour costs ($).

L can be determined from the Wessel equation :

$$L = 32 \cdot N \cdot C^{0.24} \tag{94}$$

where N = the number of steps or departments that constitute the plant (-)
C = the capacity of the plant (kT/a)

Substituting these equations in the simplified model the model becomes:

$$K_T = a \cdot k_p \cdot P + f \cdot I + d \cdot 32 \cdot N \cdot C^{0.24} \tag{95}$$

Substituting the "Beste model" values the following is obtained:

$$K_T = 1.13 \cdot k_p \cdot P + 0.13 \cdot I + (26 \cdot 32) \cdot N \cdot C^{0.24} \tag{96}$$

aflossing; niet afschrijving

The "Beste model" factor f has to be corrected, since interest and depreciation have not been taken in consideration. This correction is called the Capital Charge. The project-duration and interest are taken to be resp. 15 years and 6%. According to table IV-9[14] the additional correction factor is 10.3%, and the factor f becomes 0.233 [0.13 + 0.103].

$$K_T = 1.13 \cdot k_p \cdot P + 0.233 \cdot I + 83.2 \cdot N \cdot C^{0.24} \tag{97}$$

or

$$K_T = K'_P + K'_I + K'_L \tag{98}$$

Remark: the constants d and to a lesser extend f can hardly be considered as constants, since they differ to much per venture and product. In the scope of the preliminary design it is sufficient to consider d and f as if they were constants.

The calculation of the production costs can be found in appendix 7A . The results of this calculation are given in table 19.

Table 19: *Results of the production costs calculation for the Taylor, Miller and Zevnik-Buchanon method.*

Cost		**Taylor**	**Miller**	**Zevnik-Buchanon**
Production depenedent costs (M$)	K'_P	22.6	22.6	22.6
Labour dependent costs (M$)	K'_L	0.8	0.8	0.8
Investment dependent costs (M$)	K'_I	20.3	17.1	18.1
Total production costs (M$)	K_t	46.7	43.4	44.5

7.2 The investment costs

The total investments can be divided in four groups:
- I_B, investments in the process units, the on site investments or battery limits (including indirect investments for construction and engineering).
- I_H, investments in aid apparatus (including indirect investments for I_H).
- I_L, the investment in abstracts, such as licences, know-how, pre-operational costs and start-up costs.
- I_W, work costs, provisions, cash and sites.

The sum of I_B and I_H is often descibed as the fixed capital, I_F.
For all the methods used for economic calculations I_F is assumed to be 75 % of the total investment costs, I_T. This assumption is based on the fact that according to the PEP-yearbook[19] economic calculations for a production capacity of this size (100,000 T/a) are conducted in this manner.

The investments (I) of the project generally depend on the capacity (G), the quality (Q) and the size (O):

$$I = f(G, Q, O) \tag{99}$$

where G is foremost dependent on the production capacity (P), Q is a reflection of the requirements a product or process has to satisfy and O is dependent on the number of elements (N) (process steps, modifications and important equipments), or sub-systems (i), (off-sites or general precautions) of the plant.
? To calculate these investments modular and non-modular methods can be used. The non-modular method is applied when the investments are assumed to be equal. If this is not the case the modular method is applied.
The modular and non-modular methods can be subdivided into two models:

1. The exponential model, in which the production capacity (P) is of significant importance.
2. The factor model, in which the equipment costs play a major role.

In this process design the investment cost calculations have been limited to the fixed capital, I_F.
Tree methods have been used to calculate I_F :
- Taylor's method (a modular exponent model),
- Miller's method (a non-modular factor model),
- Zevnik-Buchanon's method (a modular exponent model).

7.3 Taylor's method

The investment costs are determined by:

$$I_B\ (k\$) = 93f*P^{0.39}*\frac{C_I}{300} \tag{100}$$

and:

$$f = \sum_{1}^{N} (1,\ 3)^{S_i} \tag{101}$$

where f = the costliness index (-)
N = the number of process steps (-)
S_i = the score of process steps (-)
P = the capacity (kT/a)
C_I = index from EPE (-)

Apart from influences of temperature, pressure and choice of materials, the calculation of the costliness index, f also takes the relative conversion of the process step into account (given as t/t product). S_I is determined according to table III-2(Montfoort 1991)[14].

The total investment costs can be determined by:

$$I_T\ (\$) = \frac{1}{0.75}*I_B\ (\$) \tag{102}$$

The results of Taylor's method are given in appendix 7B.

- The calculated costliness index f is 46.2.
- The production capacity is 100 kT/a.
- The index from EPE can be estimated from price indices from the years 1990 to 1995 (Webci and Wubo, 1994) and EPE-indices Table III-53 (Montfoort, 1991). The price indices for (January) 1990 (a key year) and 1995 are, respectively, 104 and 116, while the EPE-index for 1990 is 680. So the EPE-index for 1995 becomes 759 (= 116/104*680).
- The total investment costs according to Taylor then become 87,335 k$.

7.4 Miller's method

Miller's method (Montfoort, 1991)[14], dating back to 1965, has a greater degree of sophistication than the 1947 method of Lang. Based on the method of Lang, it is a more accurate method for calculating I_F, as aspects are considered in more detail in this method. It is based on a "four-area concept", which means it divides the plant into the following four sectors:

- The Process Installation (PI) (also called the battery limit)
- Utilities (U) (gas, air, water, electricity etc.)
- Storage and Handling (S & H) and
- Services (S) (laboratories, offices, roads, canteens etc.)

The PI investment has to be calculated first. Thereafter, the U, S & H and S investments can be calculated as percentages of the PI investment. The PI investment is based on modified Lang factors (LF). LFs, in turn, are based on the average cost of apparatus in the PI. The crux of modified LFs is that they are dependent on a combination of dimensions of apparatus, construction materials and operating pressures. Miller has established a relationship between LFs and the average cost of apparatus. The latter is defined as the total costs of apparatus in the PI divided by the number of apparatus installed.

The following sub-sections present results of calculations involved. The actual methods of calculation, further details and explanations, regarding the attainment of the results can be found in appendix 7B.

7.4.1 Calculation of the PI investment

The PI investment can be calculated with the aid of Tables III-36 and III-37 (Montfoort, 1991). In order to use these tables, however, the Average Unit Cost (AUC) of the PI has to be determined first. The AUC of the PI has been calculated based on prices shown in table 20. These prices are pertaining to 1995 and have been obtained from the PEP Yearbook[22]. However, the Miller method is based on the 1958 AUC. In order to convert the 1995 AUC to 1958 AUC, the Chemical Engeneers Plant Cost Index (USA) column, in Table III-53 (Montfoort, 1991) has been used. Based on this column, the AUC of the PI obtained in 1995 divided by a factor 4 gives a satisfactory estimate of the corresponding AUC in 1958.

Table 20: *Estimate of the AUC of the PI from the various unit-costs of the PI*

Unit	Unit cost in k$	Unit	Unit cost in k$
C1	10.7	H8	416.0
C2	42.7	H9	78.0
E1	17.8	H10	93.5
E2	19.3	H11	57.4
GLS1	19.6	P1	27.5
GLS2	2.1	P2	26.7
H1	57.4	P3	14.9
H2	505.6	R1(a,b,c)	242.0
H3	78.5	S1	146.3
H4	65.0	T1	291.1
H5	102.0	T2	1,500.8
H6	141.0	T3	172.3
H7	314.0	V1	7.4
Regenerator			195.5
Estimated AUC (k$)			**172.0**

what has been done here?

From the 1995 AUC the 1958 AUC of the PI is 172.0/4 = 43.0 k$.

From table III-36[14] is obtained that an AUC of 43.0 k$ the process is in the category over 17,000 $. In the table below, a number of factors for estimating battery limit costs are stated. An overview of the nature of different costs is presented, magnitudes of costs involving the PI investments are stated.

Table 21: *Overview of the different costs*

NATURE OF COST	CATEGORISING OF COST *(categorised as 4 different types: low, average, high or very high, unless specified otherwise)*	COSTS ($)
BASIC EQUIPMENT (delivered to site, excluding sales, taxes and catalyst)		
• AUC	Average Unit Cost	43,000
	Basic Equipment Cost (BEC) = AUC	43,000
FIELD ERECTION OF BASIC EQUIPMENT	average; 13 % of BEC; [8 - 13 % of BEC]	5,590
EQUIPMENT FOUNDATIONS AND STRUCTURAL SUPPORTS	high; 14.5 % of BEC; [13 - 15.5 % of BEC]	6,235
PIPING (includes duct-work, excludes insulation)	high; 10.5 % of BEC; [6 - 10.5 % of BEC]	4,515
INSULATION OF EQUIPMENT ONLY	average; 2.2 % of BEC; [0.8 - 2.2 % of BEC]	946
INSULATION OF PIPING ONLY	average; 4.0 % of BEC; [2 - 4 % of BEC]	1,720
ALL ELECTRICAL (except building lightning and instrumentation)	Chemical plants; 6.0 % of BEC; [2.5 - 6 % of BEC]	2,580
INSTRUMENTATION	Miscellaneous; 8 % of BEC; [2 - 8 % of BEC]	3,440
MISCELLANEOUS (includes site preparation, painting and other factors not accounted for above)	large; 6.0 % of BEC; [1 - 6 % of BEC]	2,580
BUILDINGS: ARCHITECTURAL & STRUCTURAL COST (BASC) (excludes building services)	Calculated builiding class = -1; Most process units not in buildings, quality of construction = low; Equipment material mostly carbon steel; Pressures are intermediate. 36 % of BEC; [21 -36 % of BEC]	15,480
BUILDING SERVICES These include:	Normal; 55 % of BASC;	8,514
• compressed air	• 1.5 % of BASC	
• electric lightning	• 18 % of BASC	
• sprinklers	• 10 % of BASC	
• plumbing	• 20 % of BASC	
• heating	• 8 % of BASC	
• ventilation with air conditioning	• 0 % of BASC	
The calculated PI investments for 1958 (PI_{1958})		94,600
The calculated PI investments for 1995 (PI_{1995}) = 4 × PI_{1958}		378,400

7.4.2 Calculation of the Utilities Investment

The Utilities Investment (UI) can be calculated from table III-32. The plant utilities and their respective costs are listed in the following table. The costs are given as UI_{1995}. The UI_{1995} is given as a percentage of the battery limit cost. It is assumed that the plant is built from grass roots.

Table 22: *Overview plant utilities and their respective costs*

Nature of cost	Classification of cost (in % of PI_{1995})	Costs (\$)
Buildings	10 [3 - 10]	37,840
Compressed air system	4 [0.1 - 4]	15,136
Gas system	6 [1.5 - 6]	22,704
Sewers & drains	3.5[1.3 - 3.5]	13,244
Steam system	11 [1.5-11]	41,624
Water system	10 [1 - 10]	37,840
Miscellaneous	3 [0.5 - 3]	11,352
	Cumulation = $\sum$ = 47.5 %	
	The evaluated UI_{1995} (\$)	179,740

The utilities requirement of the butyraldehyde plant is classified as high, since the total utilities requirement is over 30 % of the PI.

7.4.3 Calculation of the Storage and Handling Investment

The Storage and Handling Investment (SHI) is classified as low. Raw materials are supplied by pipeline. There is little warehouse space, since finished products are sold immediately.
For a grassroots plant the SHI is 2 % of the PI investments. Therefore **SHI = 7,568 $**.

7.4.4 Evaluation of the Services Investment

Miller's method calculates the Services Investment (SI) as a percenatge of the cumulative value of the previous investments. The cumulative value of the PI_{1995}, UI_{1995} and the SHI_{1995} is 565,708 $. This total is known as subtotal 1 (ST1). The various services needed are listed in the following table, along with their respective values.

Table 24: *Overview of the services needed*

Nature of costs	Classification of costs (% of ST 1)	Cost (\$)
Main office	5 [1 - 5]	28,285
Laboratories	2.8 [0 - 2.8]	15,839
Lunch rooms	2.2 [0 - 2.2]	12,445
Change houses	2.2 [0 - 2.2]	12,445
Personnel and gatehouses	1.0 [0 - 1]	5,657

Nature of costs	Classification of costs (% of ST 1)	Cost (\$)
Roads, railroads and fences	5.5 [1.3 - 5.5]	31,113
Service equipment	4.5 [0.5 - 4.5]	25,456
Miscellaneous	2 [0.5 - 2]	11,314
	Cumulative = $\sum$ = 25.2 %	
	The calculated SI_{1995} (\$)	142,558

Since the SI_{1995} is more than 25 % of ST1, it classified as high.

7.4.5 The calculation of I_F

The I_F based on Miller's method is defined as

$$I_F = f \times \Sigma E_i = f \times N \times ATI \tag{103}$$

where f = Lang factor
N = total number of main plant units
ATI = Average Total Investment *per unit in the PI* estimated by Miller's method.

The Lang factor can be estimated from figure III-33. An average main plant item cost of 172 k\$ yields a Lang factor of 3.0.
The total number of plant items is 26, so

TPC $= PI_{1995} + UI_{1995} + SHI_{1995} + SI_{1995}$
$= \$\ (378,400 + 179,740 + 7,568 + 142,558) = \$\ 708,266.$

Miller's method estimates I_F to be 3.0 × 26 × \$ 708,266 = M\$ 55,245.

The total investment costs according to the Taylor method are a little over M\$ 87. I_F according to Milller is M\$ 55. The difference in the estimations obtained from both methods is due to the fact that they emphasize different aspects of cost engineering. Taylor's method of calculation is based on the production capacity, and the choice of 'functional units', which is rather arbitrary. Miller's method is based on the apparatus costs. All other investments are based on the equipement investments. This is also rather arbitrary.

7.5 The Zevnik-Buchanon Method

This method is based on the fact that the investment costs are dependent on two variables:
- the process capacity
- the process complexity

To estimate the investment costs only four basic data are required:
- the process capacity
- the number of funtional units in the process flow sheet
- the complexity factor, C_F
- the plant cost index, C_I

A functional unit is considered to be equipment including all the side equipment, which is assumed to be as expensive as the 'primairy' apparatus for the same capacity if corrected for operating conditions, such as pressure and temperature. This correction is called the complexity factor. Essential for this method is that the process must consist of ample equipment (functional units).

Procedure:

I. Estimate the maximal attainable temperature and determine the temperature factor, F_t from figure III-16 (Montfoort, 1991)

for T > 290 K:

$$F_t = 0.018 * \frac{T - 290}{100} \tag{104}$$

for T ≤ 290 K:

$$F_t = -0.20 * \frac{T - 290}{100} \tag{105}$$

II. Estimate the maximal attainable pressure in the process and determine the pressure factor, F_P, from figure III-17 (Montfoort, 1991)

III. Determine the material factor, F_m, regarding the chosen construction material from figure III-18 (Montfoort, 1991). The significance of the material on the costs is pointed out by the factor 10^{F_m}.

IV. Determine the complexity factor, C_f, from:

$$C_f = 2 * 10 * (F_t + F_p + F_m) \tag{106}$$

V. Determine the investment costs per functional unit (I_E) from figure III-20 (Montfoort, 1991). The calculation of I_E is carried out taking into account a degression factor, m, of 0.6 for processes with a production capacity of more than 4500 t/a. For smaller production capacities a degression factor, m, of 0.5 is taken.

VI. Determine the investment costs:

$$I_B + I_H = N * I_E * 1.33 * \frac{C_I}{219} \tag{107}$$

The factor 1.33 is a factor that includes extra investments for utilities and general facilities into the investment costs calculation. The factor 219 is used because back in 1978 a value for C_I of 219 was used to draw up the figures for conducting this method.

Finally equation 107 can also be described as:

$$I_B = N * 0.1 * C_f * p^m * C_I \tag{108}$$

where: I_B = investment costs (k$)
p = production capacity (kT/a)
m = degression-exponent (-)
C_I = C.E.-Plant Cost Index (-)
C_f = complexity factor (≥ 2)

To attain a more acurate result the investment costs can also be calculated for each functional unit independently. This can be done in two ways:

1. by focussing on the individual functional unit capacity and then averaging C_f:

$$I_B = 0.1 * C_f * (\sum_{i=1}^{N} p_i^{\,m}) * C_I \tag{109}$$

2. by additionally determining C_f for each functional unit:

$$I_B = 0.1 * (\sum_{i=1}^{N} C_{f_i} * p_i^{\,m}) * C_I \tag{110}$$

p_i And C_{fi} are resp. the production capacity and the complexity factor per functional unit.
This last procedure was taken to carry out the required calculations.

As in the Taylor calculations the process was considered to consist out of 7 units (3 reactors, 3 columns and a settler). The calculated I_B was 58.4 M$, and therefore the total investments 77.9 M$.

7.6 Economic Criteria

Besides technological criteria a process has to satisfy some economic criteria. An analysis of the plant's economics is done by means of comparing the exploitation result with the investments. This result can be expressed as a percentage of the investment done. The analysis is done by means of:

1 Return On Investment, **ROI**.
2 Pay-Out Time, **POT**.
3 Internal Rate of Return, **IRR**.

A distinct difference can be made between the static and dynamic methods to determine if a process meets the economical criteria. In contrast to static methods take the dynamic methods in account the project life time, the discounted cashflow and time in general. The ROI and POT are both statical methods whereas the IRR is a dynamical method.

7.6.1 Return On Investment

This method is useful for the comparison of process alternatives with equal life time and production patterns (but is not very sensitive to market information). It is therefore often used in the design stage. Some of the drawbacks of the method are that it doesn't account for:

- the lower, than the design or full, capacity in the starting phase,
- the change in the value of the corresponding currency and
- variation of the costs and proceeds in time.

ROI calculations are useful for comparing different process alternatives, but are ?
The ROI is given by deviding the profit by the total investment:

$$ROI = \frac{W_a}{I_F + I_W} \cdot 100\ \% \qquad (111)$$

where W_a = the total annual average profit made after sales (\$)
I_F = the fixed capital investments (\$)
I_W = the work-costs investments (\$)

abs. drempel. nog ge winst.

For a plant with a life time of 15 years the minimum value of the ROI is 6.67 %.

criterium?

7.6.2 Pay-Out Time

The Pay-Out Time or POT is defined as the minimum number of years necessary to regain the investments with the profit made (POT < lifetime plant). This made can be used for comparison of projects with different lifetimes, differences in the values of the cost and proceeds in time. The drawbacks of this method are that the following is not taken into consideration:

- the time-dependence of the value of money,
- the time after the POT,
- the construction time,
- the interest and sometimes taxes.

Only the capital investment is regained, since the assumption is made that working capital is returned at the termination of the project. The same goes for rest value s. The capital investment I_F is described as a negative cashflow. Therefore the POT is determined by:

$$\sum_{0}^{POT} E_o = s + I_w \qquad (112)$$

where I_w = work costs, provisions, cash and sites (\$),
s = rest value (\$).

The right parenthesis can be neglected, because usually [$s + I_W$] << I_F, which gives:

$$\sum_{0}^{POT} E_o = 0 \qquad (113)$$

or

$$\sum_{1}^{POT} E_o = I_F \qquad (114)$$

where I_F = fixed capital (\$)
E_o = exploitation excess (\$)

$$E_o = P - K_V - K_{SV} \tag{115}$$

where P = proceeds ($),
K_V = variable costs ($),
K_{SV} = semi-variable costs ($).

criterium

7.6.3 Internal Rate of Return

The different cashflows, including the investments, are calculated over the duration of the project to their present values. They are returned at a return rate r which is chosen so as that these discounted cash flows (DCFs) are zero for then duration of the project. The value of r is the economic criterium $\boxed{(> 10\,\%).}$ criterium ?
The internal rate of return r is calculated by

12 à 15

$$\sum_{0}^{n} C_f\, D_i = 0 \tag{116}$$

where C_f = cash flow ($/a)
D_i = Discrete account factor in the year I = $1/(1 + r/100)^{i}$ ←
r = IRR (%)
n = economic life time of the plant (years)

The cash flow is given by

$$C_f = P - K_T + d$$

where C_f = cash flow
P = product sales
K_T = production costs
d = depreciation

7.6.4 Results

In order to estimate if the designed process satisfies the economical criteria three methods are used: the Taylor, Miller and Zevnik-Buchanon methods. The Taylor and Miller method give higher fixed capital investments, compared to the Zevnik-Buchanon method, and therefore lower profit (Taylor 27.5 M$/a, Miller 30.8 M$/a, and Zevnik-Buchanon 29.7 M$/a). The economical criteria are shown in table 25. The calculations can be found in Appendix 7E .

Table 25: *Economical criteria.*

		Taylor	Miller	Zevnik-Buchanon
ROI	(%)	39.0	52.0	47.0
POT	(Year)	1.3	1.1	1.2
POT $_{S \text{ and } I_w \text{ included}}$	(Year)	1.5	1.3	1.4
IRR	(%)	27.5	43.6	39.0

10 %

According to the Taylor, Miller and Zevnik-Buchanon methods the designed process satisfies the economic criteria.

The Return On Investments and Internal Rate of Return calculated are rather high and the Pay-Out Times are rather short. However the design made is pure theoretical and only the basics are considered. In conducting the economic calculations fluctuations in demand and price of products or feed, mal-function of equipments or other factors which influence the process economics are not accounted for. Information in the design-phase is very limited and assumptions have to be made to to predict the missing values. The methods used to calculate the process economics make assumptions that simplify the calculations, but also limit the applicability of the method. The Zevnik-Buchanon method for example is based on the assumption that for equal conditions (pressure, temperature) and construction material any equipment represents an equal investment. The fixed capital cost can therefore be calculated with average equipment costs and a plant complexity factor, that accounts for the fact that a plant is more than just a summation of the equipments. If the plant consist of enough equipments this methods is simple and effective. The Taylor method has simular principles and the Miller method is the most sophisticated economical model. A disadvantage of the Miller method is that it requires extensive information on all equipment.

8. Conclusions and recommendations

The objectives of this preliminary design for a normal-butyraldehyde plant have been achieved. The product specifications have been met, the normal butyraldehyde produced is 99.8 w/w % pure, water content is zero. The byproduct iso-butyraldehyde is 98.46 w/w % pure. This corresponds to a 89.7 % conversion of the propylene feed to butyraldehyde, carbonmonoxide conversion is 89.7 %, hydrogen conversion is 85.6 %. The feed losses in the product streams are neglected. The production target for normal-butyraldehyde, 100,000 t/a, is achieved, the production capacity is 101,000 t/a. Iso-butyraldehyde production is minimized by proper catalyst choice. The iso-butyraldehyde production capacity is 6,001 t/a. The total fuel gas stream leaving the plant is 1,740 t/a.

The process heat management has been carried out as efficiently as possible by cooling all product streams to 36 °C, and thereby heating or preheating process streams and process feed streams, to optimize conversion and separation processes. Heat available at a high level has been recovered by generating low pressure steam.

Process off gases are sold as fuel gas, rhodium losses are negligable in comparison to ligand costs. The only sources of waste are the catalyst and the regeneration agents. The catalyst is regenerated and recycled to the reactor section and is therefore not considered as waste. Catalyst losses are minimal. The regeneration agents are considered to be waste. The only emisions are fugitive emissions from the reactor, the stripper, the distillation columns and the control valves.

The reaction section is not very sensitive to temperature fluctuations because it contains a large amount of water, which acts as a heat storage medium. Therefore it is relatively easy to ensure stable operation of the reaction section. The only possible bottleneck is the extensive stirring mechanism. The operation of the separation section is highly sensitve to temperature and pressure fluctuations. Stable operation is essential to meet product specifications.

The economic analysis of the design gives for the total investments I_T according to Taylor 87.3 M$, Miller gives 73.3 M$ and Zevnik-Buchanon gives 77.9 M$. The Pay Out Time POT for Taylor, Miller and Zevnik-Buchanon respectively are 1.5, 1.3 and 1.4 years. For the Return On Investment ROI is calculated that Taylor gives 39 %, Miller gives 52 % and Zevnik-Buchanon 47 %. Their respective Internal Rates of Return IRR are 27.5 %, 43.6 % and 39.0 %. These values can be regarded as highly optimistic.

The major bottleneck in the heat management is the low process temperature level. This leads to small temperature differences which require to large heat transfer areas and therefore complicates heat management. The low process temperature level only allows low pressure steam generation. This low temperature level is due to the high temperature sensitivity of the catalyst, which degenerates at temperatures above 120 °C. This problem can be avoided by choosing a different type of catalyst with similar selectivity and activity. This catalyst should be operated at a higher temperature. A higher temprature level may result in a gas phase process. Mixing in the gas phase is faster and more homogeneous than mixing of a gas/liquid phase system. It is therefore recommended to investigate the possibilities of designing a gas phase process, which is based on a solid state or immobilized catalyst.

Another field of investigation is the use of a continuous regeneration system. In case of a continuous regeneration system is no need for a reactor shut-down, during exchange of the batches between the regenerator and the reactor.

The stream leaving the top section of the I/lights distillation column might be condensed more eficiently using a separate cryogenic condensor cascaded with a water cooled condensor instead of using a single cryogenic condensor.

* Choice of number of reactors more critical.

9. List of symbols

Symbol	**Description**	**Dimension**
a	Production costs correction factor	-
A	Constant	-
A	Catalyst activity	mol/mol h
A	Phase interphase area	m^2
A	Heat transfer area	m^2
A_{col}	Column cross section	m^2
A_{spec}	Column specific interphase	m^2/m^3
ATI	Average total investment	$
b	Settler width	m
B	Bottom product flow rate	kmol/s
B	Constant	-
Bo	Bode number	-
BP	Atmospheric boiling point	°C
C	Plant capacity	kT/a
C_ϵ	Constant	-
C_{CD}	Constant	-
C_f	Complexity factor	-
C_f	Cash flow	$/a
C_{FL}	Flooding constant	-
C_I	EPE-index	-
C_I	C.E. plant cost index	-
C_{tr}	Capacity coefficient	-
c_w	Bubble drag coefficient	-
d	Depreciation	$
d	Constant	-
D	Distillate flowrate	kmol/s
D	Impeller diameter	m
D	Sparger diameter	m
d_b	Bubble diameter	m
D_b	Bundle diameter	mm
D_{col}	Column diameter	m
D_{eg}	Gas dispersion coefficient	m^2/s
D_G	Gasphase diffusion coeficient	m^2/s
d_i	Tube inside diameter	m
D_i	Discrete account factor in the year i	-
D_L	Liquid phase diffusion coefficient	m^2/s
d_o	Tube outside diameter	m
d_p	Nominal packing diameter	m
E_{col}	Overall column efficiency	-
E_{MV}	Murphree efficiency	-
E_O	Exploitation excess	$
E_p	Polytropic efficiency	-
f	Costliness index	-
f	Lang factor	-
f	Capital charge	-
f	Friction factor	-
F	Column feed	kmol/s
F_g	Molar gas flow rate	kmol/s
F_{LG}	Liquid-vapour flow parameter	-

F_m	Material factor	-
F_p	Packing factor	-
F_p	Pressure factor	-
Fr	Froude number	-
F_t	Temperature correction factor	-
F_t	Temperature factor	-
g	Gravitational acceleration	m/s^2
h	Settler height	m
H_B	Bottom product moalr enthalpy	kJ/kmol
h_{col}	Column height	m
H_D	Distillate molar enthalpy	kJ/kmol
H_F	Feed molar enthalpy	kJ/kmol
$H_{G,1}$	Molar vapour enthalpy	kJ/kmol
h_{nb}	Nucleate pool boiling heat transfer coefficient	W/m^2 °C
h_s	Shell-side heat transfer coefficient	W/m^2 °C
h_{sd}	Shell-side dirt heat transfer coefficient	W/m^2 °C
h_t	Tube-side heat transfer coefficient	W/m^2 °C
h_{TB}	Column height from top to bottom	m
h_{td}	Tube-side dirt heat transfer coefficient	W/m^2 °C
H_V	Bubble column height	m
H_w	Liquid phase height	m
I	Total investment costs	$/a
I_B	Investment costs	$/a
I_B	Investment costs	$
I_E	Investment costs per functional unit	$
I_F	Fixed capital	$
I_T	Total investment costs	$/a
I_W	Work capital	$
j_f	Tube-side friction factor	-
K	Molar distribution coefficient	-
K_1	Empirical constant	-
k_{12}^L	Liquid phase throughpur coefficient	-
k_{12}^V	Gasphase throughput coefficient	-
K_A	General costs	$/a
K_F	Manufacturing costs	$/a
K_O	Indirect maufacturing costs	$/a
k_{oy}	Throughput coefficient	-
k_P	Raw materials costs	$/T
K_P	Production volume dependent costs	$/a
K_{SV}	Semi-variable costs	$/a
K_T	Total costs	$/a
K_V	Variable costs	$/a
k_w	Thermal conductivity of the material	W/m °C
l	Settler length	m
L	Length of one tube	m
L	Total labour costs	$/a
L	Sparger length	m
L_0	Liquid reflux	kmol/s
L_n	Liquid flow rate feed tray	kmol/s
L_r	Liquid flow rate rectifying section	kmol/s
L_s	Liquid flow rate stripping section	kmol/s
m	Constant	-
m	Volumetric distribution coefficient	-

m	Degression exponent	-
MAC	Maximum allowable concentration	ppm
M_G	Vapour mass flow rate	kg/s
MP	Atmospheric melting point	°C
Mw_G	Vapour phase molar weight	kg/kmol
Mw_L	Liquid phase molar weight	kg/kmol
n	Economic plant lifetime	a
n	Polytropic exponent	-
N	Process number of functional units	-
N	Impeller speed	s^{-1}
n_1	Empirical constant	-
N_A	Aeration number	-
$N_{A,FL}$	Maximum aeration number at which flooding occurs	-
N_{cd}	Complete dispersion impeller speed	s^{-1}
N_{col}	Actual number of trays	-
N_{oy}	Throughput number	-
N_p	Number of tube passes	-
N_t	Number of tubes	-
P	Product sales	$/a
P	Proceeds	$/a
P	Power	kW
P	Operating pressure	Pa
P	Added stirrer power	kW
P	Plant production capacity	kT/a
p_1	Inlet pressure	Pa
p_2	Outlet pressure	Pa
P_a	Actual power	kW
P_c	Liquid critical pressure	Pa
P_g	Heat produced by gas flow	kW
Po	Power number	-
p_s	Pressure at the sparger	Pa
p_t	Pressure at the top of the column	Pa
p_t	Tube pitch	mm
P_t	Theoretical power	kW
q	Feed liquid fraction	-
q	Heat flux	W/m^2
Q	Heat transferred	W
q_c	Critical heat flux	W/m^2
Q_{con}	Condenser heat duty	kW
Q_g	Volumetric gas flow rate	m^3/s
q_i	Amount of I neede per ton of product	-
Q_L	Volumetric liquid flow rate	m^3/s
Q_{reb}	Reboiler heat duty	kW
r	IRR	%
R	Reflux ratio	-
R	Dimensionless temperature ratio	-
R	Gas constant	J/mol K
Re	Reynolds number	-
RMM	Rounded molecular mass	g/mol
s	Cross section side dimension	-
s	Rest value	$
S	Dimensionless temperature ration	-
S_i	Process step score	-

t	Water temperature	°C
t	Time	s
T	Absolute temperature	K
T	Tank diameter	m
t_1	Inlet tube-side fluid temperature	°C
T_1	Inlet shell-side fluid temperature	°C
t_2	Outlet tube-side fluid temperature	°C
T_2	Outlet shell-side fluid temperature	°C
t_c	Liquid circulation time	s
T_{in}	Inlet temperature	K
t_m	Liquid mixing time	s
T_s	Tray spacing	m
T_V	Bubble column diameter	m
u	Horizontal liquid velocity	m/s
U	Overall heat transfer coefficient	W/m^2 °C
U_0	Shell-side surface based heat transfer coefficient	W/m^2 °C
$u_{G,max}$	Maximum vapour velocity	m/s
u_G	Vapour velocity	m/s
u_t	Water velocity	m/s
u_t	Tube-side velocity	m/s
$\hat{u}_{v,max}$	Maximum shell-side vapour velocity	m/s
V	Volume	m^3
V	Voltage	V
V_t	Top tray vapour stream	kmol/s
v_b	Bubble rise velocity	m/s
v_d	Droplet settling velocity	m/s
v_g	Gas velocity	m/s
V_g	Gas volume	m^3
v_{gs}^c	Pressure corrected mean superficial gas velocity	m/s
V_i	Costs of raw material I	$/T•a
V_l	Liquid volume	m^3
V_{N+1}	Vapour flow rate on tray number 1	kmol/s
V_R	Reactor volume	m^3
v_s	Mean superficial gas velocity	m/s
V_T	Bubble column volume	m^3
V_w	Liquid phase volume	m^3
W	Work	kW/kg
W_a	Total average profit after sales	$
W_{actual}	Actual work	kW/kg
X	Constant	-
x_1	n-Butyraldehyde liquid mole fraction	-
Y	Constant	-
y_1	n-Butyraldehyde vapour mole fraction	-
Z	Compressibility factor	-

Greek

α	Constant	-
α_{LK}	Light key component relative volatility	-
β	Constant	-
δ_G	Gas phase boundary layer thickness	m
ΔH_1^{vap}	n-Butyraldehyde heat of vaporization	kJ/kmol
ΔH_2^{vap}	i-Butyraldehyde heat of vaporization	kJ/kmol

ΔH_r	Reaction enthalpy	kJ/mol
δ_L	Liquid phase boundary layer thickness	m
Δp	Wet column presure drop	Pa
ΔP	Pressure drop	Pa
Δp_d	Dry column pressure drop	Pa
ΔP_t	Tube-side pressure drop	Pa
ΔT_{lm}	Log mean temperature difference	°C
ΔT_m	Mean temperature difference	°C
ϵ	Volumetric gas holdup	m^3/m^3
η_l	Liquid viscosity	Pa s
η_o	Overall efficiency	-
ρ	Density	kg/m^3
ρ_g	Gas phase density	kg/m^3
ρ_l	Liquid phase density	kg/m^3
ρ_v	Vapour density	kg/m^3
τ	Residence time	s
τ_g	Gas residence time	s
ϕ_g	Volumetric gas flow rate	m^3/s
φ	Constant	-

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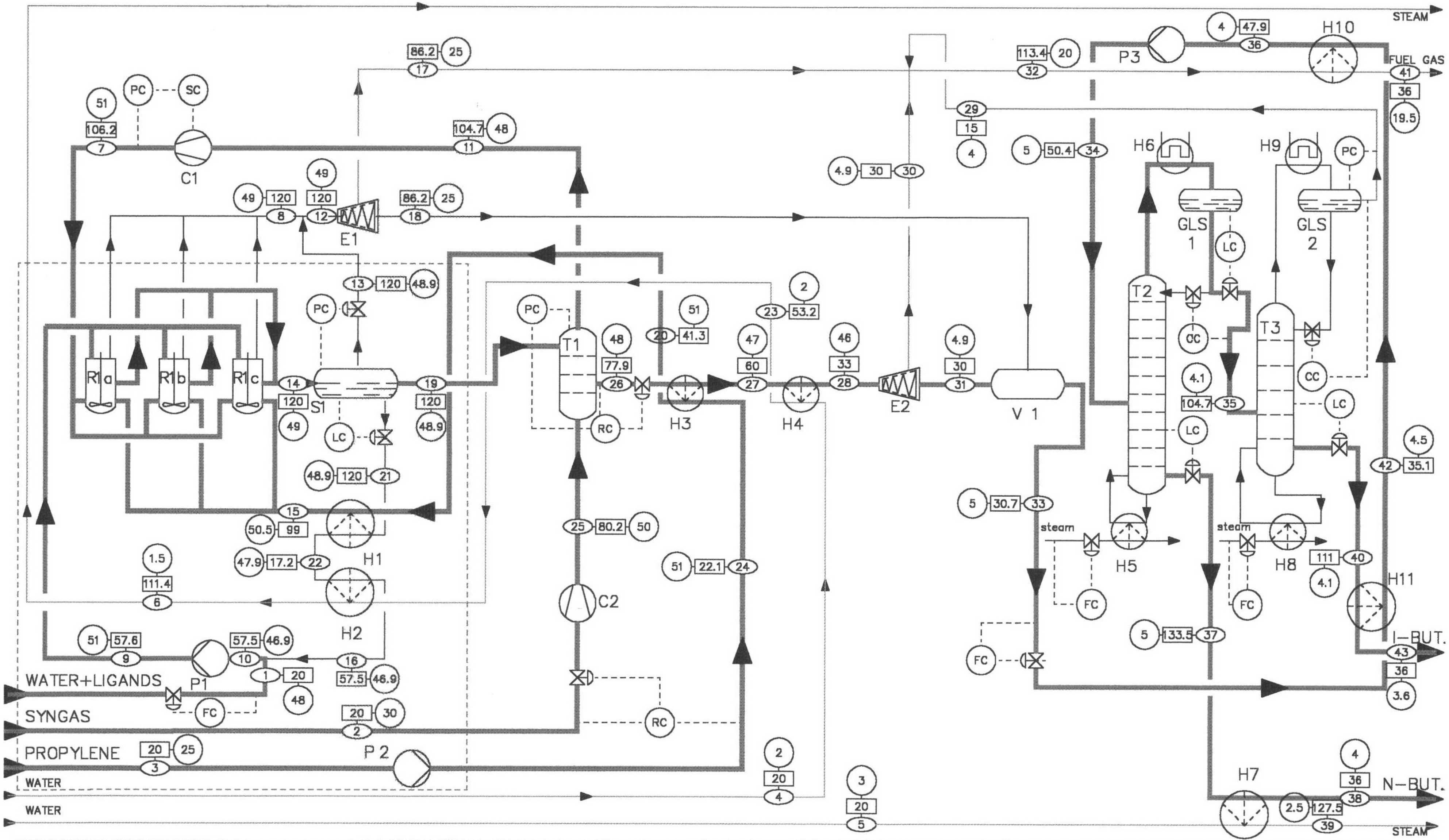
Appendices

Appendix 1

Process Flow Sheet



C1	SYNGAS COMPRESSOR	GLS2	GAS-LIQUID SEPARATOR	H5	REBOILER	H10	HTXR:FUEL GAS-PRODUCT	R1a	CSTR WITH GAS INLET	T2	N/I-DIST. COLUMN
C2	SYNGAS COMPRESSOR	H1	HTXR:WATER REC.-PROPYLENE	H6	CONDENSOR	H11	HTXR:I-BUT.-PRODUCT	R1b	CSTR WITH GAS INLET	T3	I/LIGHTS-DIST. COLUMN
E1	EXPANDER	H2	HTXR:WATER REC.-WATER	H7	HTXR:N-BUT.-WATER	P1	PUMP	R1c	CSTR WITH GAS INLET	V1	VESSEL
E2	EXPANDER	H3	HTXR:PRODUCT-PROPYLENE	H8	REBOILER	P2	PUMP	S1	3-PHASE SETTLER		
GLS1	GAS-LIQUID SEPARATOR	H4	HTXR:PRODUCT-WATER	H9	CONDENSOR	P3	PUMP	T1	STRIPPER		

MAIN STREAM — *WATER/STEAM*
FUEL GAS — *ZOOM IN FOR PROCESS CONTROL*
WATER RECYCLE

streamnr. (nr.) — pressure (bar) (P) — temperature (C) [T]

PROCESS FLOWSHEET FOR THE PRODUCTION OF N/I-BUTYRALDEHYDE

FVO 3186 SEPTEMBER 1996

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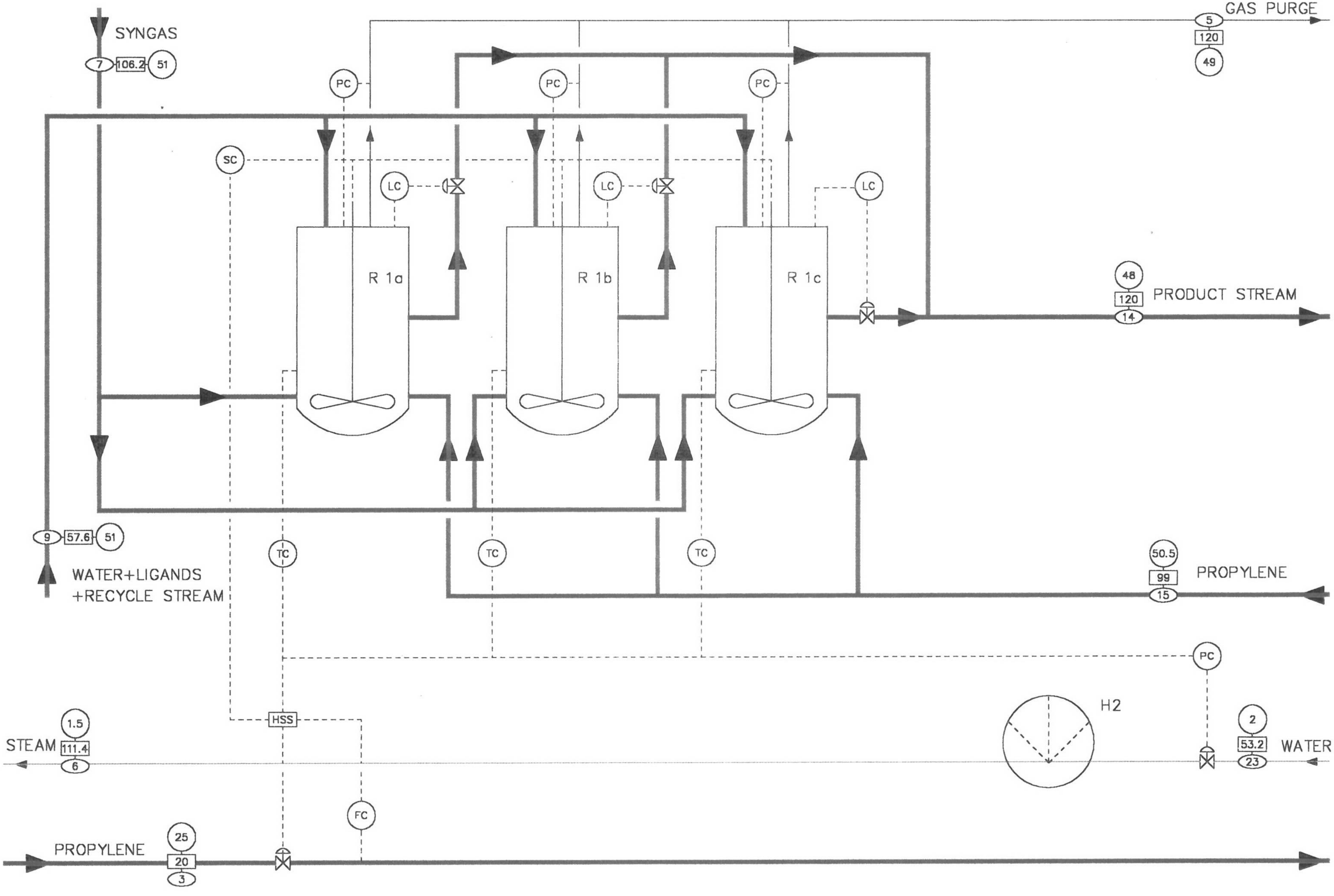
ZOOM IN ON REACTOR SYSTEM FOR PROCESS CONTROL



Appendix 2
Equipment Specifications

Appendix 2: Equipment specifications

A. Equipment Specifications for Compressors/Expanders

FVO Nr. 3188

APPARAAT NO.	C1	C2	E1	E2
Benaming: **Type:**	Compressor	Compressor	Expander	Expander
Te verpompen medium :	synthesis gas	enriched synthesis gas	reactor and settler gaseffluent	stripper effluent
Capaciteit : [t/d]/[kg/s]	1.76	3.55	0.32	1.87
Dichtheid gas in [kg/m³] :	34.3	17.6	38.8	43.2
Dichtheid gas uit [kg/m³]:	36.1	24.0	20.3	9.9
Dichtheid vloeistof in [kg/m³]			-	783.0
Dichtheid vloeistof uit: [kg/m³]:			674.7	787.3
Pin :	30	48.0	45.0	46.0
Puit :	50	51.0	25.0	4.9
Temp. In [°C]:	20	104.7	120.0	33.0
Temp. Uit	80	106.2	86.2	30.0
Vermogen [kW]				
- theorie:				
- praktijk:	266.7	46.9	-18.5	-158.1
Aantal				
- serie:				
- parallel:				
Speciale constructie-materialen				
Overig: **Netto vermogen verbruik [kW]:**	137			

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FVO Nr. : 3188

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B. HEATEXCHANGER SPECIFICATIONS

APPARAATNUMMER: H 1

Aantal serie:
Aantal parallel :

Algemene eigenschappen

Type:
~~- warmtewisselaar~~
~~- koeler~~
~~- condensor~~
*** verdamper**

Uitvoering:
~~- met vaste pijpplaten~~
~~- floating head~~
*** haarspeld**
~~- dubbele pijp~~
~~- platenwarmtewisselaar~~

Positie:
*** horizontaal**
~~- verticaal~~

Capaciteit:	**325.4**	**[kW] (berekend)**
Warmtewisselend oppervlak:	**5.5**	**[m^2] (berekend)**
Overall warmteoverdrachts-coëfficiënt:	**1260**	**[W/m^2.K] (globaal)**
Logaritmisch temperatuursverschil (LMTD):	**47.2**	**[°C]**
Aantal passages pijpzijde:	**2**	
Aantal passages mantelzijde:	**1**	
Correctiefactor LMTD (min. 0.75):	**1.0**	
Gecorrigeerde LMTD: [°C]	**47.2**	

Bedrijfscondities

		Mantelzijde	**Pijpzijde**
Soort fluïdum		water en liganden	propylene
Massastroom	**[kg/s]**	27.47	2.45
Massastroom te			
- verdampen	**[kg/s]**	0.0	0.0
- condenseren	**[kg/s]**	0.0	0.0
Gemiddelde soortelijke warmte	**[kJ/kg.°C]**	4.25	2.91
Verdampingswarmte	**[kJ/kg]**	0.0	83.0
Temperatuur IN	**[°C]**	120.0	53.0
Temperatuur UIT	**[°C]**	118.1	99.0
Druk	**[bar]**	48.9	51.0
Materiaal		Stainless steel	Stainless steel

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APPARAATNUMMER: H 2

Aantal serie:
Aantal parallel :

Algemene eigenschappen

Type:
*** warmtewisselaar**
~~- koeler~~
~~- condensor~~
~~- verdamper~~

Uitvoering:
- ~~met vaste pijpplaten~~
~~- floating head~~
*** haarspeld**
~~- dubbele pijp~~
~~- platenwarmtewisselaar~~

Positie:
*** horizontaal**
~~- verticaal~~

Capaciteit:	**6.9e3**	**[kW] (berekend)**
Warmtewisselend oppervlak:	**312**	**[m^2] (berekend)**
Overall warmteoverdrachts-coëfficiënt:	**2000**	**[$W/m^2.K$] (globaal)**
Logaritmisch temperatuursverschil (LMTD):	**11**	**[°C]**
Aantal passages pijpzijde:	**2**	
Aantal passages mantelzijde:	**1**	
Correctiefactor LMTD (min. 0.75):	**1.0**	
Gecorrigeerde LMTD: [°C]	**11.0**	

Bedrijfscondities

		Mantelzijde	**Pijpzijde**
Soort fluïdum		water en liganden	water / stoom
Massastroom	**[kg/s]**	27.47	2.76
Massastroom te			
- verdampen	**[kg/s]**	0.0	2.70
- condenseren	**[kg/s]**	0.0	0.0
Gemiddelde soortelijke warmte	**[kJ/kg.°C]**	4.22	4.2
Verdampingswarmte	**[kJ/kg]**	0.0	2540
Temperatuur IN	**[°C]**	117.9	41.3
Temperatuur UIT	**[°C]**	58.5	111.4
Druk	**[bar]**	47.9	2.0
Materiaal		stainless steel	stainless steel

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APPARAATNUMMER: H 3

Aantal serie:
Aantal parallel :

Algemene eigenschappen

Type:	*** warmtewisselaar** ~~- koeler~~ ~~- condensor~~ ~~- verdamper~~
Uitvoering:	~~- met vaste pijpplaten~~ ~~- floating head~~ *** haarspeld** ~~- dubbele pijp~~ ~~- platenwarmtewisselaar~~
Positie:	*** horizontaal** ~~- verticaal~~

Capaciteit:	**192.9**	**[kW]**	**(berekend)**
Warmtewisselend oppervlak:	**20.9**	**[m^2]**	**(berekend)**
Overall warmteoverdrachts-coëfficiënt:	**300**	**[$W/m^2.K$]**	**(globaal)**
Logaritmisch temperatuursverschil (LMTD):	**30.8**	**[°C]**	
Aantal passages pijpzijde:	**2**		
Aantal passages mantelzijde:	**1**		
Correctiefactor LMTD (min. 0.75):	**1.0**		
Gecorrigeerde LMTD: [°C]	**30.8**		

Bedrijfscondities

		Mantelzijde	**Pijpzijde**
Soort fluïdum		ongezuiverd butyraldehyde uit stripper	propylene
Massastroom	**[kg/s]**	3.75	2.45
Massastroom te			
- verdampen	**[kg/s]**	0.0	0.0
- condenseren	**[kg/s]**	0.0	0.0
Gemiddelde soortelijke warmte	**[kJ/kg.°C]**	2.77	4.16
Verdampingswarmte	**[kJ/kg]**	0.0	0.0
Temperatuur IN	**[°C]**	77.9	22.1
Temperatuur UIT	**[°C]**	60.0	53.2
Druk	**[bar]**	48.5	52.0
Materiaal		Stainless steel	Stainless steel

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APPARAATNUMMER: H 4

Aantal serie:
Aantal parallel :

Algemene eigenschappen

Type:	*** warmtewisselaar** ~~- koeler~~ ~~- condensor~~ ~~- verdamper~~
Uitvoering:	~~- met vaste pijpplaten~~ ~~- floating head~~ *** haarspeld** - ~~dubbele pijp~~ ~~- platenwarmtewisselaar~~
Positie:	*** horizontaal** - ~~verticaal~~

Capaciteit:	246.1	[kW]	(berekend)
Warmtewisselend oppervlak:	13.7	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt:	750.0	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD):	24	[°C]	
Aantal passages pijpzijde:	2		
Aantal passages mantelzijde:	1		
Correctiefactor LMTD (min. 0.75):	1.0		
Gecorrigeerde LMTD: [°C]	24.0		

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		ongezuiverd butyraldehyde	water
Massastroom	[kg/s]	3.75	2.75
Massastroom te			
- verdampen	[kg/s]	0.0	0.0
- condenseren	[kg/s]	0.0	0.0
Gemiddelde soortelijke warmte	[kJ/kg.°C]	2.31	4.2
Verdampingswarmte	[kJ/kg]	0.0	0.0
Temperatuur IN	[°C]	88.8	20.0
Temperatuur UIT	[°C]	41.3	33.0
Druk	[bar]	46.0	2
Materiaal		Stainless steel	Stainless steel

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APPARAATNUMMER: H 7

Aantal serie:
Aantal parallel :

Algemene eigenschappen

Type:
- *** warmtewisselaar**
- ~~- koeler~~
- ~~- condensor~~
- ~~- verdamper~~

Uitvoering:
- ~~- met vaste pijpplaten~~
- ~~- floating head~~
- *** haarspeld**
- \- ~~dubbele pijp~~
- \- ~~platenwarmtewisselaar~~

Positie:
- *** horizontaal**
- \- ~~verticaal~~

Capaciteit:	**1000 [kW] (berekend)**
Warmtewisselend oppervlak:	**131.4 [m^2] (berekend)**
Overall warmteoverdrachts-coëfficiënt:	**750 [$W/m^2.K$] (globaal)**
Logaritmisch temperatuursverschil (LMTD):	**10.2 [°C]**
Aantal passages pijpzijde:	**2**
Aantal passages mantelzijde:	**1**
Correctiefactor LMTD (min. 0.75):	**1.0**
Gecorrigeerde LMTD: [°C]	**10.2**

Bedrijfscondities

		Mantelzijde	**Pijpzijde**
Soort fluïdum		n-butyraldehyde	water
Massastroom	**[kg/s]**	3.47	0.38
Massastroom te			
- verdampen	**[kg/s]**	0.0	0.0
- condenseren	**[kg/s]**	0.0	0.0
Gemiddelde soortelijke warmte	**[kJ/kg.°C]**	2.35	4.2
Verdampingswarmte	**[kJ/kg]**	0.0	2210
Temperatuur IN	**[°C]**	133.5	20.0
Temperatuur UIT	**[°C]**	36.0	127.5
Druk	**[bar]**	4.5	2.5
Materiaal		Stainless steel	Stainless steel

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APPARAATNUMMER: H 10

Aantal serie:
Aantal parallel :

Algemene eigenschappen

Type:
*** warmtewisselaar**
~~- koeler~~
~~- condensor~~
~~- verdamper~~

Uitvoering:
- ~~met vaste pijpplaten~~
- ~~floating head~~
*** haarspeld**
~~- dubbele pijp~~
~~- platenwarmtewisselaar~~

Positie:
*** horizontaal**
~~- verticaal~~

Capaciteit:	**113.5**	**[kW]**	**(berekend)**
Warmtewisselend oppervlak:	**25.1**	**[m^2]**	**(berekend)**
Overall warmteoverdrachts-coëfficiënt:	**300**	**[W/m^2.K]**	**(globaal)**
Logaritmisch temperatuursverschil (LMTD):	**15.1**	**[°C]**	
Aantal passages pijpzijde:	**2**		
Aantal passages mantelzijde:	**1**		
Correctiefactor LMTD (min. 0.75):	**1.0**		
Gecorrigeerde LMTD: [°C]	**15.1**		

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		fuel gas	ongezuiverd butyraldehyde naar kolom
Massastroom	**[kg/s]**	0.54	3.70
Massastroom te			
- verdampen	**[kg/s]**	0.0	0.0
- condenseren	**[kg/s]**	0.0	0.0
Gemiddelde soortelijke warmte	**[kJ/kg.°C]**	3.88	2.32
Verdampingswarmte	**[kJ/kg]**	0.0	0.0
Temperatuur IN	**[°C]**	113.4	35.1
Temperatuur UIT	**[°C]**	36.0	47.9
Druk	**[bar]**	22.0	4.5
Materiaal		Stainless steel	Stainless steel

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APPARAATNUMMER: H 11

Aantal serie:
Aantal parallel :

Algemene eigenschappen

Type:	*** warmtewisselaar** ~~- koeler~~ ~~- condensor~~ ~~- verdamper~~
Uitvoering:	~~- met vaste pijpplaten~~ ~~- floating head~~ *** haarspeld** ~~- dubbele pijp~~ - ~~platenwarmtewisselaar~~
Positie:	*** horizontaal** ~~- verticaal~~

Capaciteit:	**38.2 [kW] (berekend)**
Warmtewisselend oppervlak:	**4.8 [m^2] (berekend)**
Overall warmteoverdrachts-coëfficiënt:	**1200 [$W/m^2.K$] (globaal)**
Logaritmisch temperatuursverschil (LMTD):	**45.3 [°C]**
Aantal passages pijpzijde:	**2**
Aantal passages mantelzijde:	**1**
Correctiefactor LMTD (min. 0.75):	**1.0**
Gecorrigeerde LMTD: [°C]	**45.3**

Bedrijfscondities

		Mantelzijde	**Pijpzijde**
Soort fluïdum		iso-butyraldehyde	ongezuiverd butyraldehyde
Massastroom	**[kg/s]**	0.21	3.70
Massastroom te			
- verdampen	**[kg/s]**	0.0	0.0
- condenseren	**[kg/s]**	0.0	0.0
Gemiddelde soortelijke warmte	**[kJ/kg.°C]**	2.40	2.33
Verdampingswarmte	**[kJ/kg]**	0.0	0.0
Temperatuur IN	**[°C]**	111.0	30.7
Temperatuur UIT	**[°C]**	36.0	35.1
Druk	**[bar]**	3.8	4.4
Materiaal		Stainless steel	Stainless steel

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C. PUMP SPECIFICATIONS

PROCESS UNIT NUMBER: P1

Dienst:
Type:
Number:

Fysical data pumpfluid

Fluid:	**water and catalyst**				
Temperature (T):	**58.4**	**[°C]**			
Density (ρ):	**983.9**	**[kg/m^3]**			
Viscosity (η):	**0.49e-3**	**[N.s/m^2]**			
Vapour pressure (p_d):	**0.182**	**[bar]**	**at temperature (T):**	**58**	**[°C]**

Power

Capacity (Φ_v):	**0.03**	**[m^3/s]**
Zuigdruk (p_z):	**45**	**[bar]**
Persdruk (p_p):	**51**	**[bar]**
Theoretical power:	**16.76**	**[kW]**
$\{ = \Phi_v \cdot (p_p - p_z).10^2 \}$		
pump efficiency:	**0.75**	**[ ]**
Axis Power:	**22.35**	**[kW]**

Construction data

Rotations per minute:	
Aandrijving:	
Type electromotor:	**'EX'N**
Voltage:	**[V]**
Direction of rotation:	
Fundationplate:	**combined/ two parts**
Elastic koppeling:	**yes/no**
Manometer suction side:	**yes/no**
Manometer pers side:	**yes/no**
Min. Excess pressure above:	
p_d/p_m:	**[bar]**

Nominal diameter zuigaansluiting:	**[ ]**
Nominal diameter persaansluiting:	**[ ]**
Lagercooling:	**ja/nee**
Packing bus cooling:	**ja/nee**
Smothering gland:	**ja/nee**
if yes:	
- dichtingsvloeistof:	**ja/nee**
- spatringen:	**ja/nee**
- packing, type:	
- sleepringafdichting:	**ja/nee**
- N.P.S.H.:	**[m]**
$\{ = p_m \cdot \rho \cdot g \}$	

Material

Pomp-huis:	**AISI 316**
Waaier:	
As:	
Bijzondere voor zieningen:	
Werkdruk:	**[bar]**

Slijtringen:	
Asbus:	
Persdruk:	**[bar]**

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PROCESS UNIT NUMBER: P2

Dienst:
Type:
Number:

Fysical data pumpfluid

Fluid: propylene feed
Temperature (T): 21.0 [°C]
Density (ρ): 511.2 [kg/m^3]
Viscosity (η): 0.09e-3 [$N.s/m^2$]
Vapour pressure (p_d): 10.6 [bar] at temperature (T): 20 [°C]

Power

Capacity (Φ_v): 4.8e-3 [m^3/s]
Zuigdruk (p_z): 25 [bar]
Persdruk (p_p): 51 [bar]

Theoretical power: 14.9 [kW]
$\{ = \Phi_v \cdot (p_p - p_z) . 10^2 \}$

pump efficiency: 0.75 [ ]
Axis Power: 19.90 [kW]

Construction data

Rotations per minute:
Aandrijving:
Type electromotor: 'EX'E
Spanning: [V]
Direction of rotation:
Fundatieplate: combined/ two parts
Elastic koppeling: yes/no
Manometer zuigzijde: yes/no
Manometer drukzijde: yes/no
Min. Overdruk boven:
p_d/p_m: [bar]

Nominal diameter zuigaansluiting: [ ]
Nominal diameter persaansluiting: [ ]
Lagerkoeling: ja/nee
Pakkingsbuskoeling: ja/nee
Smothering gland: ja/nee
if yes:
- dichtingsvloeistof: ja/nee
- spatringen: ja/nee
- packing, type:
- sleepringafdichting: ja/nee
- N.P.S.H.: [m]
$\{ = p_m . \rho . g \}$

Material

Pomp-huis: AISI 316
Waaier:
As:
Bijzondere voor zieningen:

Werkdruk: [bar]

Slijtringen:
Asbus:

Persdruk: [bar]

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PROCESS UNIT NUMBER: P3

Dienst:
Type:
Number:

Fysical data pumpfluid

Fluid:	**productstream to distillation column, mainly butyraldehyde**				
Temperature (T):	47.9	[°C]			
Density (ρ):	764.8	[kg/m^3]			
Viscosity (η):	0.34e-3	[N.s/m^2]			
Vapour pressure (p_d):	0.73	[bar]	**at temperature (T):**	50	[°C]

Power

Capacity (Φ_v):	4.62e-3	[m^3/s]
Zuigdruk (p_z):	4	[bar]
Persdruk (p_p):	5	[bar]
Theoretical power: $\{ = \Phi_v.(p_p - p_z).10^2 \}$	0.46	[kW]
pump efficiency:	0.75	[ ]
Axis Power:	0.62	[kW]

Construction data

Rotations per minute:		**Nominal diameter zuigaansluiting:**	[ ]
Aandrijving:		**Nominal diameter persaansluiting:**	[ ]
Type electromotor:	'EX'E	**Lagercooling:**	ja/nee
Voltage:	[V]	**Packing bus cooling:**	ja/nee
Direction of rotation:		**Smothering gland:**	ja/nee
Fundationplate:	combined/ two parts	**if yes:**	
Elastic koppeling:	yes/no	**- dichtingsvloeistof:**	ja/nee
Manometer suction side:	yes/no	**- spatringen:**	ja/nee
Manometer pers side:	yes/no	**- packing, type:**	
Min. Excess pressure above:		**- sleepringafdichting:**	ja/nee
p_d/p_m: [bar]		**- N.P.S.H.:** $\{ = p_m.\rho.g \}$	[m]

Material

Pomp-huis:	AISI 316	**Slijtringen:**	
Waaier:		**Asbus:**	
As:			
Bijzondere voor zieningen:			
Werkdruk:	[bar]	**Persdruk:**	[bar]

D. REACTORS, SETTLER AND VESSEL SPECIFICATIONS

APPARAAT NO.	R1a, R1b, R1c				
Benaming: **Type:**	CSTR with gasinlet	Settler	Stripper	Mixing vessel	
Abs./Eff. druk [bar] :	50	49	48	5.0	
Temp. [°C] :	120	120	77.9	30.7	
Inhoud $[m^3]$:	40	90			
Diameter [m] :	2.94	11	0.75		
L of H [m] :	5.88	3.7 bij 2.2	7.0		
Vulling :		n.v.t.	n.v.t.		
Schotels (+ aantal) :	n.v.t.	n.v.t.	Sieve Tray (3)		
Vaste pakking:	n.v.t.	n.v.t.	n.v.t.		
Kat. type:	Rhodium with TPPTS as ligand	n.v.t.	n.v.t.		
Kat. vorm:		n.v.t.	n.v.t.		
Speciale constructie-materialen	mechanical seal for the stirrer	nee	nee		
Aantal in					
- serie:					
- parallel:	3				
Overig:					

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E. COLUMN SPECIFICATIONS

APPARAATNUMMER: T1: Stripper

Algemene eigenschappen

Functie = ~~destillatie~~ / **extractie** / ~~absorptie~~

Type toren = ~~gepakt~~/ **schotel** / ~~sproeier~~

Type schotel = ~~klokje /~~ **zeefplaat** /~~valve~~
Aantal schotels
- theoretisch =
- practisch = **3**
- Voedingschotel(pract) = **1 en 3**
Schotelafstand (HETS) = **2.3** [m] **Materiaal schotel:** **Stainless steel**
Diameter toren = **0.84** [m] **Hoogte toren:** 7.0 [m]
Materiaal toren = **Steel H II**
Verwarming = **geen** /~~open stoom / reboiler~~

Bedrijfscondities

	Voeding	**Top**	**Bodem**	**Reflux-/ Absorptie-middel**	**Extractie-middel**
Temp. [°C]		104.7	77.9		
Druk [bar]		48	48		
Dichtheid liquid [kg/m^3]		602.45	703.33		
Dichtheid gas [kg/m^3]		34.12	26.78		
Massastroom [kg/s]		8.03	5.86		

	mol%	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	
Samenstelling:									
propylene			1.73	2.08	0.11	0.14			
carbon monoxide			27.41	21.94	33.85	29.55			
hydrogen			30.22	1.73	35.39	2.21			
propane			10.27	12.92	0.715	0.98			
water			0.77	0.397	0.06	0.04			
n-butyraldehyde			27.73	57.09	28.1	63.09			
isobutyraldehyde			1.86	3.83	1.77	3.97			

Ontwerp

Aantal klokjes / zeefgaten:

Actief schoteloppervlak: **0.30 [m^2]**

Lengte overlooprand: [mm]

Diameter valpijp / gat: [mm]

Type pakking:
Materiaal pakking:
Afmetingen pakking
- inhoud: [m^3]
- lengte: [m]
- breedte: [m]
- hoogte: [m]

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr.:3188
Datum: / /
Ontwerpers:
R.M. Lenz
C.A.A. Schuurmans
G.A. Pouw
E.V. Verhoef

APPARAATNUMMER: T2: N / Iso-butyraldehyde distillatie

Algemene eigenschappen

Functie = **destillatie** ~~/ extractie / absorptie~~

Type toren = ~~gepakt~~ **/ schotel /** ~~sproeier~~

Type schotel = ~~klokje~~ **/ zeefplaat /** ~~valve~~
Aantal schotels
- theoretisch = **83**
- practisch = **87**
- Voedingschotel(pract) = **35**
Schotelafstand (HETS) = **0.56** [m] **Materiaal schotel:**
Diameter toren = **1.95** [m] **Hoogte toren:** 49 [m]
Materiaal toren = **Steel HII**
Verwarming = ~~geen / open stoom~~ **/ reboiler**

Bedrijfscondities

	Voeding		**Top**		**Bodem**		**Reflux-/ Absorptie-middel**		**Extractie-middel**
Temp. [°C]	127		111		133				
Druk [bar]	4.45		4.10		4.99				
Dichtheid [kg/m^3]	668		674		661				
Massastroom [kg/s]	16.3		10.4		16.7				
	mol%	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	
Samenstelling									
propylene	0.02	0.01	0.10	0.06	0	0			
carbon monoxide	0	0	0.01	0	0	0			
hydrogen	0	0	0	0	0	0			
propane	0.11	0.07	0.48	0.30	0	0			
water	0.11	0.03	1.72	0.44	0	0			
n-butyraldehyde	92.08	92.20	0.31	0.28	99.8	99.8			
isobutyraldehyde	7.67	7.69	97.39	98.92	0.2	0.2			

Ontwerp

Aantal klokjes / zeefgaten:

Actief schoteloppervlak: **1.981** [m2]

Lengte overlooprand: [mm]

Diameter gat: 6.4 [mm]

Type pakking:
Materiaal pakking:
Afmetingen pakking
- inhoud: [m^3]
- lengte: [m]
- breedte: [m]
- hoogte: [m]

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APPARAATNUMMER: T3: Iso-butyraldehyde / light ends

Algemene eigenschappen

Functie = destillatie ~~/ extractie / absorptie~~

Type toren = ~~gepakt /~~ schotel / ~~sproeier~~

Type schotel = ~~klokje /~~ zeefplaat / ~~valve~~
Aantal schotels
- theoretisch = 9
- practisch = 11
- Voedingschotel(pract) = 9
Schotelafstand (HETS) = 0.61 [m] **Materiaal schotel:** Stainless steel
Diameter toren = 0.31 [m] **Hoogte toren:** 6.7 [m]
Materiaal toren = Steel H II
Verwarming = ~~geen / open stoom /~~ reboiler

Bedrijfscondities

	Voeding		Top		Bodem		Reflux-/ Absorptie-middel		Extractie-middel
Temp. [°C]	105.95		87.85		108.41				
Druk [bar]	4.08		4.00		4.09				
Dichtheid liquid [kg/m^3]	673		687		673				
Dichtheid gas [kg/m^3]	9.14		8.05		9.35				
Massastroom [kg/s]	0.49		0.40		0.49				
	mol%	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	
Samenstelling									
propylene	0.10	0.06	6.86	4.89	0.04	0.02			
carbon monoxide	0.01	0.00	0.34	0.16	0.00	0.00			
hydrogen	0.00	0.00	0.09	0.00	0.00	0.00			
propane	0.48	0.30	38.08	28.39	0.09	0.06			
water	1.72	0.44	0.08	0.02	0.00	0.00			
n-butyraldehyde	0.31	0.28	0.05	0.06	0.45	0.46			
iso-butyraldehyde	97.39	98.92	54.50	66.48	99.42	99.46			

Ontwerp

Aantal klokjes / zeefgaten:

Actief schoteloppervlak: 0.06 [m^2]

Lengte overlooprand: [mm]

Diameter valpijp / gat: [mm]

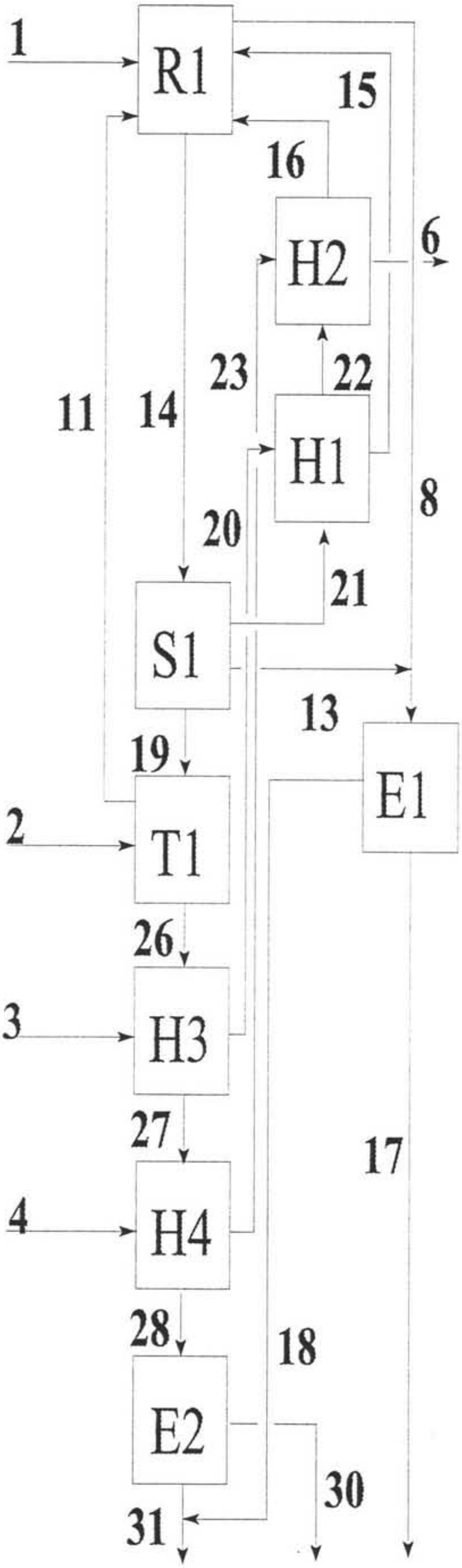
Type pakking:
Materiaal pakking:
Afmetingen pakking
- inhoud: [m^3]
- lengte: [m]
- breedte: [m]
- hoogte: [m]

Appendix 3

Mass and Heat Balance

Mass and Heat Balance

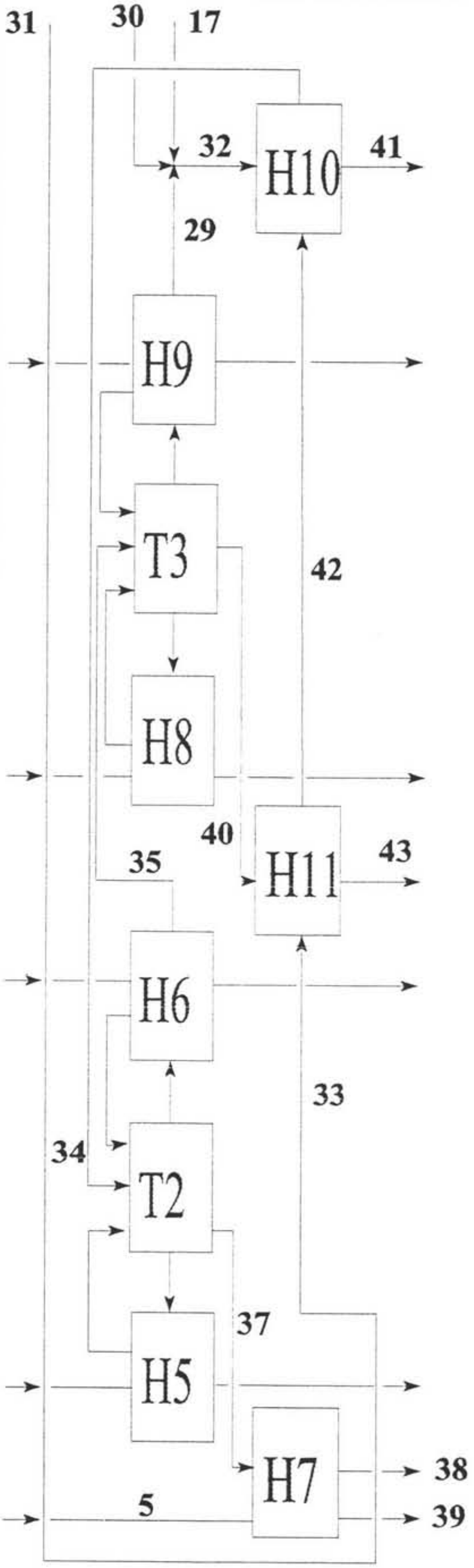
IN M In kg/s	IN Q In kJ/s	Forward M Q
0.0156 *(1)*	-245.9 *(1)*	
		0.47 *(8)*
		-1296 *(8)*
		33.01 *(14)*
		-441e3 *(14)*
		8.3e-4 *(13)*
		-2.534 *(13)*
		5.54 *(19)*
		-16378 *(19)*
1.75 *(2)*	-6595.6 *(2)*	3.75 *(26)*
		-12085 *(26)*
		0.43 *(17)*
		-1158 *(17)*
2.45 *(3)*	-146.1 *(3)*	3.75 *(27)*
		-12278 *(27)*
2.76 *(4)*	-43794 *(4)*	
		0.04 *(18)*
		-169 *(18)*
		3.75 *(28)*
		-125 *(28)*
		0.09 *(30)*
		-350 *(30)*
		3.66 *(31)*
		-12199 *(31)*



Back M Q	OUT M In kg/s	OUT Q In kJ/s
27.47 *(16)*		
-431722 *(16)*		
3.55 *(11)*	2.76 *(6)*	-36681 *(6)*
-106666 *(11)*		
2.76 *(23)*		
-43550 *(23)*		
27.47 *(22)*		
-424861 *(22)*		
2.45 *(20)*		
67 *(20)*		
27.47 *(21)*		
-424611 *(21)*		

Mass and Heat Balance

IN M In kg/s	IN Q In kJ/s	Forward M Q
		0.54 *(32)* - 1547 *(32)*
663 Koelwater	- 10.58e6	
		0.23 *(35)* - 688.3 *(35)*
		3.70 *(42)* -1661 *(42)*
13.59	- 205.4e3	
		0.21 *(40)* - 675.7 *(40)*
11.97 Koelwater	- 190e3	
		3.70 *(34)* - 12215.5 *(34)*
18.31	-276e3	
		3.47 *(37)* -12481.7 *(37)*
0.40 *(5)*	-6329.4 *(5)*	
714.23	**-11.31e6**	



TOTAL

Back M Q	OUT M In kg/s	OUT Q In kJ/s
	0.54 *(41)*	-1661 *(41)*
	663 Koelwater	- 10.47e6
	13.59	- 210.4e3
	0.21 *(43)*	-713.9 *(43)*
	11.97 Koelwater	- 194e3
	18.31	- 272e3
	3.47 *(38)*	-11547.8 *(38)*
	0.40 *(39)*	- 5276.7 *(39)*
	714.25	**-11.21e6**

Appendix 4
Dow's Fire and Explosion Index

Appendix 4: Dow's fire and explosin index

Determining the Dow's Fire and Explosion Index

To determine the Dow's Fire and Explosion Index (DFEI) a Unit Hazard Factor (F_3) and a Material Factor (MF) are required. The MF is a measure of the intensity of energy release from a chemical compound, mixture or subtance. The MF is determined by considering two hazards of a material: flammability (N_f) and reactivity (N_r) and is denoted by a number from 1 to 40. A mixture can be assigned a weighted average based on weight per cent.

The hydroformylation reactor:

The MF for the hydroformylation reactor is determined to be equal to 9.93.
The Unit Hazard Factor is calculated by reviewing the Contributing Hazards. Each of the items are considered to be a contributing factor in the development of an incident which can cause a fire or an explosion. Not every item is applicable to a given process unit. In table A4.1 the Unit Hazard Factor is determined:

Table A4.1: *Determination of the Unit Hazard Factor for the hydroformylation reactor*

	Type	Penalty
General Process Hazard	- Exothermic Reaction	0.8
	- Base Factor	1.0 +
General Hazard Factor (F_1)		1.8
Special Process Hazard	- Process Temperature	0.6
	- Relief Pressure (0.78*1.3)	1.01
	- Quantity of Flammable Material	1.25
	- Corrosion and Erosion	0.1
	- Leakage	0.3
	- Base Factor	1.0 +
Special Hazard Factor (F_2)		4.26
Unit Hazard Factor ($F_3 = F_1 * F_2$)		7.67
Fire and Explosion Index (F_3 * MF)		76.2

The stripper

The Material Factor has a value of 21.6.
The Unit Hazard Factor is determined in table A4.2

Table A4.2: *Determination of the Unit Hazard Factor of the stripper*

	Type	Penalty
General Process Hazard	-	-
	- Base Factor	1.0 +
General Hazard Factor		1.0

Special Process Hazard	- Temperature	0.6
	- Relief Pressure	0.9
	- Quantity of Flammable Materials	1.25
	- Corrosion	0.1
	- Leakage	0.1
	- Base Factor	1.0 +
Special Hazard Factor		3.95
Unit Hazard Factor		3.95
DFEI		85.32

The distillation column

The Material Factor for the n/iso-butyraldehyde column has a value of 23.9
The Unit Hazard Factor is determined in table A4.3

Table A4.3: *Determination of the Unit Hazard Factor of the n/iso butyraldehyde column*

	Type	Penalty
General Process Hazard	-	-
	- Base Factor	1.0 +
General Hazard Factor (F_1)		1.0
Special Process Hazard	- Process Temperature	0.6
	- Relief Pressure	0.19
	- Quantity of Flammable Material	0.9
	- Corrosion	0.1
	- Leakage	0.1
	- Base Factor	1.0 +
Special Hazard Factor (F_2)		2.89
Unit Hazard Factor (F_3) ($F_3 = F_1 * F_2$)		2.89
Fire and Explosion Index ($MF*F_3$)		69.1

With the MF and the Unit Hazard Factor a Damage Factor (DF) can be made.
An area of possible exposure can be made with the known DFEI.
This gives for the the following table for the three process units:

Table A4.4: *The damage factor and the area of exposure for the reactor, stripper and column*

	Reactor	Stripper	distillation column
Damage Factor	0.27	0.66	0.65
Exposure Radius [m]	19.50	21.94	17.98
Area of Exposure [m^2]	1194.60	1512.25	1015.62

This means that the stripper has a damage probability of 66% to 1512 m^2 of surrounding area and the reactor has a 27% damage probabilty to 1194 m^2 of surrounding area.

Appendix 5
Equipment Design

Appendix 5A

Distillation Column Calculation

ChemCAD data

N/l-separation

unit 10

	rectifying section		tot.col.	stripping section	
	top	*bottom*	prop.	*top*	*bottom*
Nact.	2	34	87	35	86
V1 (kmol/h)			515.23		
D (kmol/h)			12.78		
L0 (kmol/h)			502.46		
F (kmol/h)			185.88		
Vn+1 (kmol/h)			663.15		
Vd (kmol/h)			12.78		
B (kmol/h)			173.1		
q (-)			1.795782		
R (-) (mole-based)			39.329		
Hg,1 (kJ/kmol)			-222654		
Hreflux (kJ/kmol)			-234546		
Hg,d (kJ/kmol)			-193925		
Hb (kJ/kmol)			-218269		
Hf (kJ/kmol)			-236596		
Mg (kg/s)	10.066	10.591		10.595	13.2755
Ml (kg/s)	10.397	10.365		16.317	16.75
Qg (m3/s)	1.053	0.995		1.201	1.112
Ql (m3/s)	0.015	0.016		0.0244	0.0254
RHOg (kg/m3)	10.088	10.651		10.698	11.946
RHOl (kg/m3)	674.685	668.187		668.039	660.673
Ts (m)	0.5	0.5		0.5	0.5
Qcon. (kJ/h)			-1.4E+07		
Qreb. (kJ/h)			1.82E+07		
Dint.(rect.) (m)			1.829		
Dint.(strip) (m)			2.134		

Heat Calculations

Qcon. (kJ/h)			-5610003		
Qreb. (kJ/h)			9327635		

Tray Column Diameter Calculations

Flg (-)	0.1263	0.12356		0.19489	0.169661
Ctr (-)	0.081486	0.081792		0.074139	0.076771
Ug,max (m/s)	0.661394	0.642653		0.581154	0.565741
Dcol (m)	1.549551	1.569261		1.646886	1.768136
Dcol (av.)(m)			1.633458		

Tray Column Height Calculations

Ecol (%)			94.87761		
Ntheor.			82.54352		
Htb (m)			43		
Hcol (m)			49		

Packed Column Calculations

random packing: Raschig-rings

Fp (1/m)			840		
d (m)			0.02		
phi (-)	0.116496	0.127365		0.160545	0.169868
Vg (m/s)	0.265133	0.256785		0.256192	0.241101
Acol. (m2)	5.673698	5.535478		6.696984	6.588835
Dcol. (m)	2.687746	2.654805		2.92008	2.896405
Vl (m/s)	0.002644	0.00289		0.003643	0.003855
eps. (-)	0.039485	0.041904		0.048898	0.050773
dPd (mbar)	233.5063	231.2574		231.2062	228.6568
dPw (mbar)	364.8171	372.1661		406.0309	411.2456

structured packing: Mellapak 250 Y

C (-)			1		
Cg,max (-)			0.14		
Flg (-)	0.1263	0.12356		0.19489	0.169661
Csp (m/s)	0.14	0.14		0.14	0.14
Ug,max (m/s)	1.136331	1.1		1.097418	1.031687
Fsp (m/s(kg/m3)^0.5)	2.887335	2.871956		2.87153	2.852653
Dcol (m)	1.182202	1.199486		1.198481	1.309358

Murphree Efficiency

A col (m2)	2.627	2.627		3.575	3.575
Aspec.(m2)	1.981	1.981		2.689	2.689
Dg (m/s2)			0.0001		
dg (m)			0.001		
Dl (m/s2)			1E-08		
dl (m)			0.0001		
K12V (m/s)			0.1		
K12L (m/s)			0.0001		
dHvap1 (kJ/kmol)	29160	27840	34910	27830	27310
dHvap2 (kJ/kmol)	27510		33080		
x1 (-)	0.015	0.928		0.93	0.997
y1 (-)	0.011	0.903		0.906	0.996
Mw,g (g/mol)	74.25	71.93		87.2	72.15
Mw,l (g/mol)	71.67	72.08		72.08	72.11
K (-)	0.72603	0.97277		0.97354	0.99915
m (-)	0.011247	0.015474		0.018861	0.018076
alpha (-)	1.0009	1.05566		1.05578	1.059798
beta (-)	1.00066	1.05416		1.05434	1.059738
Koy (-)	0.008158	0.005751		0.004769	0.004946
Noy (-)	3.157066	2.355061		2.989159	3.348187
Emv (%)	95.74496	90.51123		94.96702	96.4852
Ecol. (%)	96.09646	91.25665		95.37977	96.77755
Ecol.tot. (%)			94.87761		

l/lights-separation

unit 16

	rectifying section		**tot.col.**	**stripping section**	
	top	*bottom*	**prop.**	*top*	*bottom*
Nact.	2	8	11	9	10
V1 (kmol/h)			12.1		
D (kmol/h)			1.55		
L0 (kmol/h)			9.74		
water decant (kmol/h)			0.8		
F (kmol/h)			12.78		
Vn+1 (kmol/h)			1.61		
Vd (kmol/h)			1.55		
B (kmol/h)			10.42		
q (-)			0.179186		
R (-) (mole-based)			6.271		
Hg,1 (kJ/kmol)			-156955		
Hreflux (kJ/kmol)			-196865		
Hg,d (kJ/kmol)			-92276.5		
Hb (kJ/kmol)			-233408		
Hf (kJ/kmol)			-193925		
Mg (kg/s)	0.233	0.256		0.027	0.031
Ml (kg/s)	0.21	0.233		0.234	0.238
Qg (m3/s)	0.0265	0.028		0.00289	0.003196
Ql (m3/s)	0.0003	0.000346		0.000348	0.000353
RHOg (kg/m3)	8.782	9.137		9.352	9.641
RHOl (kg/m3)	686.968	673.326		673.17	673.398
Ts (m)	0.5	0.5		0.5	0.5
Qcon. (kJ/h)			-378400		
Qreb. (kJ/h)			50170		
Dint.(rect.) (m)			0.305		
Dint.(strip) (m)			0.152		

Heat Calculations

Qcon. (kJ/h)	-161341
Qreb. (kJ/h)	64567.34

Tray Column Diameter Calculations

Flg (-)	0.101904	0.106024		1.021508	0.91863
Ctr (-)	0.084245	0.083774		0.033251	0.033545
Ug,max (m/s)	0.740328	0.714255		0.280144	0.278338
Dcol (m)	0.238825	0.249863		0.128071	0.135595

Tray Column Height Calculations

Ecol (%)			75		
Ntheor.			8.25		
Htb (m)			5		
Hcol (m)			11		

Packed Column Calculations

random packing: Raschig-rings

Fp (1/m)			840		
d (m)			0.02		

phi (-)	0.100126	0.106079		1.021038	0.923872
Vg (m/s)	0.28674	0.278309		0.275059	0.270951
Acol. (m2)	0.132026	0.143725		0.01501	0.016851
Dcol. (m)	0.410001	0.427781		0.138243	0.146475
Vl (m/s)	0.002272	0.002407		0.023172	0.020966
eps. (-)	0.035693	0.037095		0.167849	0.157024
dPd (mbar)	53.37412	52.3142		52.30208	52.31979
dPw (mbar)	79.65227	79.39785		745.0026	572.5622

structured packing: Mellapak 250 Y

C (-)			1		
Cg,max (-)			0.14		

Flg (-)	0.101904	0.106024		1.021508	0.91863
Csp (m/s)	0.14	0.14		0.14	0.14
Ug,max (m/s)	1.230285	1.193636		1.179506	1.16164
Fsp (m/s(kg/m3)^0.5	2.916705	2.886449		2.885643	2.88551
Dcol (m)	0.185266	0.193286		0.062416	0.066375

Stripper

unit	5

Nact.	3
D (kmol/h)	579.08
F1 (kmol/h)	337.54
F2 (kmol/h)	437.74
B (kmol/h)	196.21
Mg (kg/s)	2.113
Ml (kg/s)	4.477
Qg (m3/s)	0.078893
Ql (m3/s)	0.006662
RHOg (kg/m3)	26.783
RHOl (kg/m3)	671.997
Ts (m)	0.5
Dint. (m) [tray 1]	0.914
Dint. (m) [tray 2 & 3]	0.762

Tray Column Diameter Calculations

Flg (-)	0.422993
Ctr (-)	0.054064
Ug,max (m/s)	0.265358
Dcol (m)	0.687883

Tray Column Height Calculations

Ecol (%)	75
Ncol	2.25
Htb (m)	1
Hcol (m)	7

Packed Column Calculations

random packing: Raschig-rings

Fp (1/m)	840
d (m)	0.02

phi (-)	0.422993
Vg (m/s)	0.162394
Acol. (m2)	0.69402
Dcol. (m)	0.940029
Vl (m/s)	0.009599
eps. (-)	0.093278
dPd (mbar)	33.22514
dPw (mbar)	108.7434

structured packing: Mellapak 250 Y

C (-)	1
Cg,max (-)	0.14

Flg (-)	0.422993
Csp (m/s)	0.14
Ug,max (m/s)	0.687148
Fsp (m/s(kg/m3)^0.5	2.844919
Dcol (m)	0.427477

Appendix 5B **Heat Exchanger calculations** *Design Estimates*

equipment h2

T1	117.9	°C	number of tubes	1293	(-)
T2	58.5	°C	cross section	0.199063	m2
t1	41.3	°C	flow	0.0275	m3/s
t2	111.4	°C	tube velocity	0.138148	m/s
T_ln	11.0	°C	*Based on 16 mm tubes:*		
Q	6.9E+06	W	D_tubes	772	mm
U	2000.0	W/m2°C	D_shell	849	mm
A	312.0	m2	A	312	m2

equipment h3

T1	77.9	°C	number of tubes	87	(-)
T2	60.0	°C	cross section	0.013335	m2
t1	22.1	°C	flow	0.004678	m3/s
t2	53.2	°C	tube velocity	0.350799	m/s
T_ln	30.8	°C	*Based on 16 mm tubes:*		
Q	192880.6	W	D_tubes	227	mm
U	300.0	W/m2°C	D_shell	249	mm
A	20.9	m2	A	20.9	m2

equipment h4

T1	60.0	°C	number of tubes	57	(-)
T2	41.3	°C	cross section	0.048029	m2
t1	20.0	°C	flow	0.004678	m3/s
t2	33.0	°C	tube velocity	0.097396	m/s
T_ln	24.0	°C	*Based on 16 mm tubes:*		
Q	246111.1	W	D_tubes	187	mm
U	750.0	W/m2°C	D_shell	281	mm
A	13.7	m2	A	13.7	m2

equipment h7

T1	133.5	°C	number of tubes	545	(-)
T2	36.0	°C	cross section	0.083836	m2
t1	20.0	°C	flow	0.000417	m3/s
t2	127.5	°C	tube velocity	0.00497	m/s
T_ln	10.2	°C	*Based on 16 mm tubes:*		
Q	1.0E+06	W	D_tubes	522	mm
U	750.0	W/m2°C	D_shell	574	mm
A	131.4	m2	A	131.4	m2

equipment h11

T1	111.0	°C	number of tubes	20	(-)
T2	36.0	°C	cross section	0.003063	m2
t1	30.7	°C	flow	0.0046	m3/s
t2	35.1	°C	tube velocity	1.502041	m/s
T_ln	26.5	°C	*Based on 16 mm tubes:*		
Q	38166.7	W	D_tubes	116	mm
U	300.0	W/m2°C	D_shell	128	mm
A	4.8	m2	A	4.8	m2

equipment h10

T1	113.4	°C	number of tubes	104	(-)
T2	36.0	°C	cross section	0.016014	m2
t1	35.1	°C	flow	0.0046	m3/s
t2	47.9	°C	tube velocity	0.287243	m/s
T_ln	15.1	°C	*Based on 16 mm tubes:*		
Q	113472.2	W	D_tubes	246	mm
U	300.0	W/m2°C	D_shell	271	mm
A	25.1	m2	A	25.1	m2

equipment h1

T1	120.0	°C	number of tubes	46	(-)
T2	118.0	°C	cross section	0.01	m2
t1	53.0	°C	flow	0.0046	m3/s
t2	90.0	°C	tube velocity	0.50	m/s
T_ln	45.3	°C	*Based on 16 mm tubes:*		
Q	325416.7	W	D_tubes	170	mm
U	1200.0	W/m2°C	D_shell	187	mm
A	6.0	m2	A	6.22	m2

Remarks

* The heat transfer coefficient used in the calculations is obtained from table 12.1[8]. No temperature correction factor is used in the mean (log) temperature difference-calculations.

** A complete design of heatexchanger H1 is presented

*** T1 and T2 are resp. the inlet outlet temperatures of the shell, where t1 and t2 are resp. the inlet and outlet temperatures of the tubes.

**** the heat transfer area is first estimated with the heat transfer equation. The tube side velocity is calculated to check if such a surface is realistic.

Design estimates

Heat-exchangers on distillation towers

equipment	T13				
topstream	h6				
T1	111.0	°C	*Design*		
T2	104.7	°C	*(Based on 16 mm tubes)*		
t1	20.0	°C	D_tubes	658	mm
t2	35.0	°C	D_shell	1119	mm
T_ln	80.3	°C	number of tubes	910	(-)
Q	4.0E+06	W			
U	500.0	W/m2°C	A	100.6	m2
			length	1.4	m
			diameter	1.12	m
A	100.6	m2	(inside,shell)		

bottomstream	h5				
T1	133.4	°C	Design		
T2	133.5	°C	*(Based on 16 mm tubes)*		
t1	200.0	°C	D_tubes	408	mm
t2	199.0	°C	D_shell	694	mm
T_ln	66.0	°C	number of tubes	317	(-)
Q	5.1E+06	W			
U	1000.0	W/m2°C	A	76.5	m2
			length	1.4	m
			diameter	0.69	m
A	76.5	m2	(inside,shell)		

equipment	T15				
topstream	h9				
T1	87.9	°C	*Design*		
T2	15.0	°C	*(Based on 16 mm tubes)*		
t1	10.0	°C	D_tubes	147	mm
t2	0.0	°C	D_shell	250	mm
T_ln	28.9	°C	number of tubes	33	(-)
Q	7.6E+04	W			
U	2000.0	W/m2°C	A	2	m2
			length	0.6	m
			diameter	0.25	m
A	1.3	m2	(inside,shell)		

bottomstream	h8				
T1	108.4	°C	*Design*		
T2	111.0	°C	*(Based on 16 mm tubes)*		
t1	200.0	°C	D_tubes	355	mm
t2	199.0	°C	D_shell	604	mm
T_ln	89.8	°C	number of tubes	233	(-)
Q	5.1E+06	W			
U	1000.0	W/m2°C	A	56.2	m2
			length	1.4	m
			diameter	0.60	m
A	56.2	m2	(inside,shell)		

Alternative for T15: Combination of cryogene and water cooling

topstream	h9				
T1	87.9	°C	*Design*		
T2	35.0	°C	*(Based on 16 mm tubes)*		
t1	20.0	°C	D_tubes	201	mm
t2	30.0	°C	D_shell	342	mm
T_ln	31.8	°C	number of tubes	66	(-)
Q	7.6E+04	W			
U	750.0	W/m2°C	A	4	m2
			length	0.6	m
			diameter	0.34	m
A	3.2	m2	(inside,shell)		

Cryogene unit	h12		(topstream)		
T1	35.0	°C	*Design*		
T2	15.0	°C	*(Based on 16 mm tubes)*		
t1	0.0	°C	D_tubes	107	mm
t2	5.0	°C	D_shell	182	mm
T_ln	21.6	°C	number of tubes	17	(-)
Q	2.9E+04	W			
U	2000.0	W/m2°C	A	1	m2
			length	0.6	m
			diameter	0.18	m
A	0.7	m2	(inside,shell)		

Design heatexchanger/vaporizer propylene feed h1

data I

H_nb (w/m2 °C)	16765.52	calculated
K_l (W/m °C)	0.02619	c.p
C_pl(J/kg°C)	2912.3	c.c
RHO_l(kg/m3)	300.3958	c.c
mu_l (N s/m2)	3.45E-05	c.c
L_v (J/kg)	83010	c.c.
RHO_v (kg/m3)	127.6	c.p
T_w (°C)	118.1348	c.c
T_s (° C)	99	c.c
P_w (N/m2)	5050000	c.p
P_s (N/m2)	4800000	c.p
sigma (N/M)	0.0005	c.c
Q (J/s)	325416.7	c.c

c.c = chemcad
c.p = chemprop

h_nb (I)	16765.52	W/m2
	80% van II	
h_nb (II)	29820.39	W/m2
	29240.28	

data II

P_c	45.95759	bar	c.c
P	50.5	bar	c.c
q	59484.01	w/m2	c.c
h_nb (II)	29820.39	W/m2	calculated

Estimates

U	1260.865	w/m2	
T_ln,cor	47.17716	°C	
A (m2)	*5.470658*	6.220353	m2
Nr. of Tub	*43.97385*	50	(-)
D_tubes	552.5404	mm	
D_shell	635.4215	mm	

Latent heat *

	propane	*propylene*	
T_b,i	*231.05*	*225.35*	*°C*
T_c,i	*369.8*	*365*	*°C*
T	*363.15*	*363.15*	*°C*
L_v,b	*18786*	*18422*	*kJ/kmol*
L_v,i	*5921.858*	*3562.431*	*kJ/kmol*
L_v	*5804.421*	*kJ/kmol*	*3501 (c.c.)*

Maximum critical flux

q_c (I)	4075564	W/m2
q_c (II)	1795744	W/m2
q	59484.01	W/m2

Overall heat-transfer coefficient

U_staal	51884.48	w/m2
propane/ propylene- foulingcoe	3000	w/m2
water foulingcoe	5000	w/m2
h_nb (II)	16765.52	w/m2
h_water	7218.323	w/m2
overall U	1260.865	w/m2

surface	0.010053	m2
flow	0.027492	m3/s
U_water	2.734647	m/s
T_water	118.1348	°C
h_water	7218.323	w/m2

Layout

Liquid level	378.0758	mm
width at liquid level:	0.605163	m
surface area liquid:	1.452392	m2
vapour surface vel.	0.013213	m/s
max. allowable vel.	0.23274	m/s

Corrected log mean T diff.

R	20.28886	
S	0.038583	
F_t	0.97708	
T_ln	48.2838	°C
T_ln,cor	47.17716	°C

Pressure drop

Re	178556.4	
J_f	0.003	
delta P_t	17620.22	pa

viscosity	6.18E-05	kg/m s
A	5.470658	m2
delta P_s	35000	pa

Design of heat exchanger h4

triangular pitch (1.25 do)	0.0625	m
length	1.3	m
diameter (internal, shell)	0.55254	m
tube diameter	0.018	m
tube thickness	0.002	m
external heat-transfer area	6.220353	m2
construction material:	stainless steel	

pressure drop tubeside	0.176202	bar
pressure drop shellside	0.35	bar
number of tubes	50	

design is based on a Kettler boiler

* the calculated latent heat is not used, but is included for completeness. The calculated heat is about half the value, given by ChemCad.

Appendix 5C

Pump design

equipment p1

flow 98934.53 kg/h
100.578 m3/h
delta P 6 bar
P_in 46.9 bar
T_in 58.4853 °C
Estimate of pump-efficiency:
0.75 _

15 % of the total power is lost to the fluid.
10 % of the total power to the surroundings.

density 983.6597 kg/m3
mean heat capacity
4183.333 J/kgK

Theoretical power.
*P_t = Flow(m)*delta P / density*
*= Flow(v)*delta P*
P_t 16763 J/s

Power
P_p 22350.67 J/s

Calculated power (Chemcad)
P_p,c 22365.4 J/s

Power-loss to fluid
P_loss,f 3352.6 J/s
Delta T 0.029162 °C
T_uit 58.51446

Power-loss to surroundings
P_loss,s 4917.147 J/s

equipment p3

flow 13310.21 kg/h 17.53073
16.633 m3/h
delta P 1 bar
P_in 5 bar
T_in 47.9359 °C
Estimate of pump-efficiency:
0.75 _

15 % of the total power is lost to the fluid.
10 % of the total power to the surroundings.

density 759.2505 kg/m3
mean heat capacity
1405.532 J/kgK

Theoretical power.
*P_t = Flow(m)*delta P / density*
*= Flow(v)*delta P*
462.0278 J/s

Power
P_p 616.037 J/s

Calculated power (Chemcad)
P_p,c 603.34 J/s

Power-loss to fluid
P_loss,f 92.40556 J/s
Delta T 0.017782 °C
T_uit 47.95368

Power-loss to surroundings
P_loss,s 135.5281 J/s

equipment p2

flow 8815.469 kg/h
17.33035 m3/h
delta P 31 bar
P_in 20 bar
T_in 20 °C
Estimate of pump-efficiency:
0.75 _

15 % of the total power is lost to the fluid.
10 % of the total power to the surroundings.

density 508.6724 kg/m3
mean heat capacity
135.7143 J/kgK

Theoretical power.
*P_t = Flow(m)*delta P / density*
*= Flow(v)*delta P*
14923.35 J/s

Power
P_p 19897.81 J/s

Calculated power (Chemcad)
P_p,c 19801.5 J/s

Power-loss to fluid
P_loss,f 2984.671 J/s
Delta T 8.981067 °C
T_uit 28.98107

Power-loss to surroundings
P_loss,s 4377.517 J/s

Appendix 6

Stream & Equipment Summary

APPENDIX 6

Stream & Equipment summary

STREAMS

Stream Summary

Stream No.	1	2	3	4	5	6	7	8	9
- - Overall - -									
Molar flow kmol/h	3.1102	437.7448	209.0116	551.1277	79.6517	551.1277	579.0759	69.4716	5491.6862
Mass flow kg/h	56.0302	6322.2192	8815.4694	9928.5656	1434.9260	9928.5656	12788.6355	1697.8341	98932.7271
Temp C	40.0000	20.0000	20.0000	20.0000	20.0000	111.3873	106.1844	120.0000	58.6217
Pres bar	48.0000	30.0000	20.0000	2.0000	3.0000	1.5000	51.0000	49.0000	51.0000
Vapor mole fraction	0.0000	1.0000	0.0000	0.0000	0.0000	0.9826	1.0000	1.0000	0.0000
Enth MJ/h	-885.0550	-23743.7000	-525.8710	-157662.0000	-22786.2000	-132054.0000	-38252.7000	-4665.5300	-1555050.0000
Tc C	374.2000	-183.3161	91.8759	374.2000	374.2000	374.2000	-38.1873	24.4790	374.2000
Pc bar	221.1823	37.6154	45.9710	221.1823	221.1823	221.1823	115.5806	122.4665	221.1823
Std. sp gr , wtr = 1	1.0000	0.4550	0.5210	1.0000	1.0000	1.0000	0.5150	0.4830	1.0000
Std. sp gr , air = 1	0.6220	0.4990	1.4560	0.6220	0.6220	0.6220	0.7630	0.8440	0.6220
Degree API	10.0110	179.6068	139.9739	10.0110	10.0110	10.0110	143.1708	161.5124	10.0110
Average mol wt	18.0150	14.4427	42.1769	18.0150	18.0150	18.0150	22.0846	24.4393	18.0150
Actual dens kg/m3	991.9615	17.5876	511.5129	997.8444	997.8444	0.8703	36.1034	38.8161	983.6449
Actual vol m3/h	0.0565	359.4696	17.2341	9.9500	1.4380	11407.9487	354.2222	43.7405	100.5777
Std liq m3/h	0.0561	13.9128	16.9282	9.9383	1.4363	9.9383	24.8469	3.5190	99.0299
Std vap 0 C m3/h	69.7109	9811.4582	4684.7134	12352.7828	1785.2859	12352.7828	12979.2027	1557.1111	123088.7165
- - Vapor only - -									
Molar flow kmol/h		437.7448				541.5517	579.0759	69.4716	
Mass flow kg/h		6322.2192				9756.0533	12788.6355	1697.8341	
Average mol wt		14.4427				18.0150	22.0846	24.4393	
Actual dens kg/m3		17.5876				0.8552	36.1034	38.8161	
Actual vol m3/h		359.4696				11407.7673	354.2222	43.7405	
Std liq m3/h		13.9128				9.7656	24.8469	3.5190	
Std vap 0 C m3/h		9811.4582				12138.1481	12979.2027	1557.1111	
Cp kJ/kmol-K		28.3557				34.2543	43.3294	54.5089	
Z factor		1.0109				0.9884	0.9893	0.9439	
Visc kg/m-s		0.0000				0.0000	0.0000	0.0000	
Th cond W/m-K		0.0776				0.0259	0.0686	0.0670	
- - Liquid only - -									
Molar flow kmol/h	3.1102		209.0116	551.1277	79.6517	9.5760			5491.6862
Mass flow kg/h	56.0302		8815.4694	9928.5656	1434.9260	172.5123			98932.7271
Average mol wt	18.0150		42.1769	18.0150	18.0150	18.0150			18.0150
Actual dens kg/m3	991.9615		511.5129	997.8444	997.8444	949.2902			983.6449
Actual vol m3/h	0.0565		17.2341	9.9500	1.4380	0.1817			100.5777
Std liq m3/h	0.0561		16.9282	9.9383	1.4363	0.1727			99.0299
Std vap 0 C m3/h	69.7109		4684.7134	12352.7828	1785.2859	214.6341			123088.7165
Cp kJ/kmol-K	75.2573		102.5933	75.4781	75.4858	76.3031			75.2936
Z factor	0.0443		0.0722	0.0019	0.0029	0.0012			0.0450
Visc kg/m-s	0.0007		0.0001	0.0010	0.0010	0.0002			0.0005
Th cond W/m-K	0.6257		0.1021	0.5990	0.5990	0.6806			0.6461
Surf tens N/m	0.0695		0.0075	0.0730	0.0730	0.0564			0.0662

Stream No.	10	11	12	13	14	15	16	17	18
- - Overall - -									
Molar flow kmol/h	5491.6862	579.0759	69.6073	0.1357	5826.2505	209.0116	5488.5762	66.9564	2.6509
Mass flow kg/h	98932.7271	12788.6355	1701.1538	3.3199	118839.0464	8815.4694	98876.6942	1561.0396	140.1143
Temp C	58.4853	104.6661	120.0027	120.0000	120.0000	90.0000	58.5000	86.2139	86.2139
Pres bar	46.9000	48.0000	49.0000	48.9000	49.0000	50.5000	46.9000	25.0000	25.0000
Vapor mole fraction	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000
Enth MJ/h	-1555100.0000	-38399.4000	-4674.6500	-9.1251	-1587590.0000	1111.9000	-1554220.0000	-4167.3800	-609.0580
Tc C	374.2000	-38.1873	24.4792	24.6238	343.7763	91.8759	374.2000	10.2370	245.7167
Pc bar	221.1823	115.5806	122.4665	122.4556	163.8964	45.9710	221.1823	118.0339	62.4768
Std. sp gr , wtr = 1	1.0000	0.5150	0.4830	0.4830	0.9380	0.5210	1.0000	0.4670	0.7810
Std. sp gr , air = 1	0.6220	0.7630	0.8440	0.8450	0.7040	1.4560	0.6220	0.8050	1.8250
Degree API	10.0110	143.1708	161.5123	161.3981	19.2940	139.9739	10.0110	171.5518	49.6599
Average mol wt	18.0150	22.0846	24.4393	24.4592	20.3972	42.1769	18.0150	23.3143	52.8552
Actual dens kg/m3	983.7144	34.3446	38.8158	38.7717	810.1625	300.3958	983.7069	20.2609	674.6744
Actual vol m3/h	100.5706	372.3621	43.8263	0.0856	146.6855	29.3462	100.5144	77.0468	0.2077
Std liq m3/h	99.0299	24.8469	3.5259	0.0069	126.7592	16.9282	98.9739	3.3463	0.1795
Std vap 0 C m3/h	123088.7165	12979.2027	1560.1534	3.0422	130587.5272	4684.7134	123019.0146	1500.7367	59.4166
- - Vapor only - -									
Molar flow kmol/h		579.0759	69.6073	0.1357				66.9564	
Mass flow kg/h		12788.6355	1701.1538	3.3199				1561.0396	
Average mol wt		22.0846	24.4393	24.4592				23.3143	
Actual dens kg/m3		34.3446	38.8158	38.7717				20.2609	
Actual vol m3/h		372.3621	43.8263	0.0856				77.0468	
Std liq m3/h		24.8469	3.5259	0.0069				3.3463	
Std vap 0 C m3/h		12979.2027	1560.1534	3.0422				1500.7367	
Cp kJ/kmol-K		43.2507	54.5118	54.5460				50.4726	
Z factor		0.9827	0.9439	0.9439				0.9629	
Visc kg/m-s		0.0000	0.0000	0.0000				0.0000	
Th cond W/m-K		0.0683	0.0670	0.0669				0.0628	
- - Liquid only - -									
Molar flow kmol/h	5491.6862				5826.2505	209.0116	5488.5762		2.6509
Mass flow kg/h	98932.7271				118839.0464	8815.4694	98876.6942		140.1143
Average mol wt	18.0150				20.3972	42.1769	18.0150		52.8552
Actual dens kg/m3	983.7144				810.1625	300.3958	983.7069		674.6744
Actual vol m3/h	100.5706				146.6855	29.3462	100.5144		0.2077
Std liq m3/h	99.0299				126.7592	16.9282	98.9739		0.1795
Std vap 0 C m3/h	123088.7165				130587.5272	4684.7134	123019.0146		59.4166
Cp kJ/kmol-K	75.2936				84.3629	122.8303	75.3363		163.5179
Z factor	0.0414				0.0460	0.2435	0.0414		0.0766
Visc kg/m-s	0.0005				0.0002	0.0000	0.0005		0.0002
Th cond W/m-K	0.6459				0.4235	0.0729	0.6460		0.1269
Surf tens N/m	0.0662				0.0303	0.0005	0.0662		0.0121

Stream No.	19	20	21	22	23	24	25	26	27
- - Overall - -									
Molar flow kmol/h	337.5385	209.0116	5488.5762	5488.5762	551.1277	209.0116	437.7448	196.2073	196.2073
Mass flow kg/h	19959.0423	8815.4694	98876.6942	98876.6942	9928.5656	8815.4694	6322.2192	13492.6260	13492.6260
Temp C	120.0000	54.3049	120.0000	117.9268	41.3395	23.3124	80.2069	77.8645	60.0000
Pres bar	48.9000	51.0000	48.9000	47.9000	2.0000	51.0000	50.0000	48.0000	47.0000
Vapor mole fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0648
Enth MJ/h	-58959.0000	239.7790	-1528620.0000	-1529500.0000	-156777.0000	-454.5850	-22946.5000	-43505.9000	-44200.3000
Tc C	205.7915	91.8759	374.2000	374.2000	374.2000	91.8759	-183.3161	240.8758	240.8758
Pc bar	62.3595	45.9710	221.1823	221.1823	221.1823	45.9710	37.6154	49.8410	49.8410
Std. sp gr , wtr = 1	0.7190	0.5210	1.0000	1.0000	1.0000	0.5210	0.4550	0.8020	0.8020
Std. sp gr , air = 1	2.0420	1.4560	0.6220	0.6220	0.6220	1.4560	0.4990	2.3740	2.3740
Degree API	65.2584	139.9739	10.0110	10.0110	10.0110	139.9739	179.6068	44.9912	44.9912
Average mol wt	59.1312	42.1769	18.0150	18.0150	18.0150	42.1769	14.4427	68.7672	68.7672
Actual dens kg/m3	477.9364	444.4716	942.4920	944.1555	991.4473	505.8320	24.0199	703.3326	537.8373
Actual vol m3/h	41.7609	19.8336	104.9098	104.7250	10.0142	17.4277	263.2076	19.1838	25.0868
Std liq m3/h	27.7785	16.9282	98.9739	98.9739	9.9383	16.9282	13.9128	16.8444	16.8444
Std vap 0 C m3/h	7565.4685	4684.7134	123019.0146	123019.0146	12352.7828	4684.7134	9811.4582	4397.7218	4397.7218
- - Vapor only - -									
Molar flow kmol/h							437.7448		12.7115
Mass flow kg/h							6322.2192		314.8399
Average mol wt							14.4427		24.7680
Actual dens kg/m3							24.0199		41.6170
Actual vol m3/h							263.2076		7.5652
Std liq m3/h							13.9128		0.4500
Std vap 0 C m3/h							9811.4582		284.9124
Cp kJ/kmol-K							28.9197		31.0379
Z factor							1.0234		1.0100
Visc kg/m-s							0.0000		0.0000
Th cond W/m-K							0.0901		0.0430
- - Liquid only - -									
Molar flow kmol/h	337.5385	209.0116	5488.5762	5488.5762	551.1277	209.0116		196.2073	183.4958
Mass flow kg/h	19959.0423	8815.4694	98876.6942	98876.6942	9928.5656	8815.4694		13492.6260	13177.7861
Average mol wt	59.1312	42.1769	18.0150	18.0150	18.0150	42.1769		68.7672	71.8152
Actual dens kg/m3	477.9364	444.4716	942.4920	944.1555	991.4472	505.8319		703.3326	752.0864
Actual vol m3/h	41.7609	19.8336	104.9098	104.7250	10.0142	17.4277		19.1838	17.5216
Std liq m3/h	27.7785	16.9282	98.9739	98.9739	9.9383	16.9282		16.8444	16.3944
Std vap 0 C m3/h	7565.4685	4684.7134	123019.0146	123019.0146	12352.7828	4684.7134		4397.7218	4112.8096
Cp kJ/kmol-K	212.7433	111.2336	76.5321	76.4435	75.2575	103.3241		190.7168	184.0987
Z factor	0.1841	0.1871	0.0386	0.0379	0.0018	0.1794		0.1608	0.1973
Visc kg/m-s	0.0001	0.0001	0.0002	0.0002	0.0007	0.0001		0.0002	0.0003
Th cond W/m-K	0.0893	0.0877	0.6831	0.6826	0.6273	0.1007		0.1227	0.1344
Surf tens N/m	0.0039	0.0034	0.0548	0.0552	0.0693	0.0071		0.0144	0.0191

Stream No.	28	29	30	31	32	33	34	35	36
- - Overall - -									
Molar flow kmol/h	196.2073	1.5533	12.9795	183.2278	81.4892	185.8787	185.8787	12.7778	185.8787
Mass flow kg/h	13492.6260	68.2769	322.5253	13170.1005	1951.8416	13310.2145	13310.2145	828.4275	13310.2145
Temp C	33.0000	15.0100	29.9744	29.9744	113.4187	30.6865	48.0536	104.7090	47.9359
Pres bar	46.0000		4.9000	4.9000	22.0000	5.0000	5.0000	4.1000	4.0000
Vapor mole fraction	0.0634	1.0000	1.0000	0.0000	0.0000	0.0001	0.0001	1.0000	0.0002
Enth MJ/h	-45086.2000	-143.3380	-1260.3100	-43917.4000	-5571.0200	-44526.4000	-43976.4000	-2478.0400	-43980.4000
Tc C	240.8758	97.8438	-123.9835	250.0208	-3.8439	249.9747	249.9747	222.8008	249.9747
Pc bar	49.8410	47.1336	64.7084	40.3302	115.7212	40.9058	40.9058	51.0592	40.9058
Std. sp gr , wtr = 1	0.8020	0.5200	0.7010	0.8050	0.4960	0.8040	0.8040	0.7630	0.8040
Std. sp gr , air = 1	2.3740	1.5180	0.8580	2.4820	0.8270	2.4720	2.4720	2.2390	2.4720
Degree API	44.9912	140.4217	70.4015	44.3689	153.7486	44.4246	44.4246	53.9016	44.4246
Average mol wt	68.7672	43.9564	24.8488	71.8783	23.9522	71.6070	71.6070	64.8332	71.6070
Actual dens kg/m3	567.3018	7.8857	9.8693	787.2988	222.4014	783.1355	761.0053	9.2034	757.4304
Actual vol m3/h	23.7839	8.6583	32.6798	16.7282	8.7762	16.9961	17.4903	90.0137	17.5729
Std liq m3/h	16.8444	0.1313	0.4606	16.3838	3.9383	16.5633	16.5633	1.0864	16.5633
Std vap 0 C m3/h	4397.7218	34.8148	290.9181	4106.8042	1826.4695	4166.2200	4166.2200	286.3978	4166.2200
- - Vapor only - -									
Molar flow kmol/h	12.4426	1.5533	12.9795			0.0135	0.0236	12.7778	0.0319
Mass flow kg/h	299.9052	68.2769	322.5253			0.3193	0.6310	828.4275	0.8974
Average mol wt	24.1031	43.9564	24.8488			23.6453	26.7309	64.8332	28.1222
Actual dens kg/m3	43.2426	7.8857	9.8693			4.6882	5.0241	9.2034	4.2330
Actual vol m3/h	6.9354	8.6583	32.6798			0.0681	0.1256	90.0137	0.2120
Std liq m3/h	0.4306	0.1313	0.4606			0.0005	0.0009	1.0864	0.0013
Std vap 0 C m3/h	278.8838	34.8148	290.9181			0.3027	0.5291	286.3978	0.7152
Cp kJ/kmol-K	29.7055	70.0916	30.8361			33.2526	37.5147	108.8680	39.5658
Z factor	1.0074	0.9308	0.9991			0.9984	0.9963	0.9195	0.9956
Visc kg/m-s	0.0000	0.0000	0.0000			0.0000	0.0000	0.0000	0.0000
Th cond W/m-K	0.0413	0.0175	0.0379			0.0442	0.0403	0.0201	0.0380
- - Liquid only - -									
Molar flow kmol/h	183.7647			183.2278	81.4892	185.8652	185.8551		185.8468
Mass flow kg/h	13192.7208			13170.1005	1951.8416	13309.8952	13309.5835		13309.3171
Average mol wt	71.7914			71.8783	23.9522	71.6105	71.6127		71.6144
Actual dens kg/m3	783.0230			787.2988	222.4014	786.2675	766.4733		766.6275
Actual vol m3/h	16.8484			16.7282	8.7762	16.9279	17.3647		17.3609
Std liq m3/h	16.4138			16.3838	3.9383	16.5628	16.5624		16.5620
Std vap 0 C m3/h	4118.8384			4106.8042	1826.4695	4165.9174	4165.6913		4165.5050
Cp kJ/kmol-K	166.8807			165.5870	92.9754	165.4853	175.3446		175.2707
Z factor	0.2032			0.0448	0.0094	0.0223	0.0216		0.0173
Visc kg/m-s	0.0004			0.0004	0.0000	0.0004	0.0003		0.0003
Th cond W/m-K	0.1419			0.1430	0.0615	0.1429	0.1380		0.1380
Surf tens N/m	0.0226			0.0231	0.0004	0.0230	0.0207		0.0207

Stream No.	37	38	39	40	41	42	43
- - Overall - -							
Molar flow kmol/h	173.0999	173.0999	79.6517	10.4222	81.4892	185.8787	10.4222
Mass flow kg/h	12481.7165	12481.7165	1434.9260	745.6956	1951.8416	13310.2145	745.6956
Temp C	133.5177	30.0000	127.4665	111.0209	36.0000	35.1276	36.0000
Pres bar	5.0000	4.0000	2.5000	4.1000	21.5000	4.5000	3.6000
Vapor mole fraction	0.0000	0.0000	1.0000	0.0000	0.9177	0.0001	0.0000
Enth MJ/h	-37782.4000	-41572.4000	-18996.1000	-2432.6100	-5979.6000	-44388.9000	-2570.1100
Tc C	251.8113	251.8113	374.2000	233.9779	-3.8439	249.9747	233.9779
Pc bar	40.0021	40.0021	221.1823	42.0441	115.7212	40.9058	42.0441
Std. sp gr , wtr = 1	0.8070	0.8070	1.0000	0.7930	0.4960	0.8040	0.7930
Std. sp gr , air = 1	2.4900	2.4900	0.6220	2.4700	0.8270	2.4720	2.4700
Degree API	43.7956	43.7956	10.0110	46.8305	153.7486	44.4246	46.8305
Average mol wt	72.1070	72.1070	18.0150	71.5490	23.9522	71.6070	71.5490
Actual dens kg/m3	660.5386	790.1026	1.3761	672.6645	22.3259	776.0450	769.6344
Actual vol m3/h	18.8963	15.7976	1042.7394	1.1086	87.4252	17.1513	0.9689
Std liq m3/h	15.4768	15.4768	1.4363	0.9406	3.9383	16.5633	0.9406
Std vap 0 C m3/h	3879.8004	3879.8004	1785.2859	233.5988	1826.4695	4166.2200	233.5988
- - Vapor only - -							
Molar flow kmol/h			79.6517		74.7809	0.0204	
Mass flow kg/h			1434.9260		1606.8103	0.5065	
Average mol wt			18.0150		21.4869	24.8734	
Actual dens kg/m3			1.3761		18.4799	4.3774	
Actual vol m3/h			1042.7394		86.9489	0.1157	
Std liq m3/h			1.4363		3.4793	0.0008	
Std vap 0 C m3/h			1785.2859		1676.1155	0.4564	
Cp kJ/kmol-K			34.2857		41.6107	34.7349	
Z factor			0.9827		0.9727	0.9977	
Visc kg/m-s			0.0000		0.0000	0.0000	
Th cond W/m-K			0.0273		0.0567	0.0421	
- - Liquid only - -							
Molar flow kmol/h	173.0999	173.0999		10.4222	6.7083	185.8584	10.4222
Mass flow kg/h	12481.7165	12481.7165		745.6956	345.0313	13309.7080	745.6956
Average mol wt	72.1070	72.1070		71.5490	51.4347	71.6121	71.5490
Actual dens kg/m3	660.5386	790.1027		672.6645	724.5070	781.2862	769.6344
Actual vol m3/h	18.8963	15.7976		1.1086	0.4762	17.0356	0.9689
Std liq m3/h	15.4768	15.4768		0.9406	0.4590	16.5626	0.9406
Std vap 0 C m3/h	3879.8004	3879.8004		233.5988	150.3540	4165.7634	233.5988
Cp kJ/kmol-K	279.3698	165.9279		183.8125	133.3424	167.7393	167.8229
Z factor	0.0201	0.0180		0.0159	0.0700	0.0199	0.0151
Visc kg/m-s	0.0002	0.0004		0.0002	0.0004	0.0004	0.0004
Th cond W/m-K	0.1174	0.1433		0.0835	0.1393	0.1416	0.1416
Surf tens N/m	0.0106	0.0235		0.0105	0.0186	0.0224	0.0190

Stream No.	1	2	3	4	5	6	7	8	9
Temp C	40.0000	20.0000	20.0000	20.0000	20.0000	111.3873	106.1844	120.0000	58.6217
Pres bar	48.0000	30.0000	20.0000	2.0000	3.0000	1.5000	51.0000	49.0000	51.0000
Enth MJ/h	-885.0600	-23744.0000	-525.8700	-157660.0000	-22786.0000	-132050.0000	-38253.0000	-4665.5000	-1555000.0000
Vapor mass fraction	0.0000	1.0000	0.0000	0.0000	0.0000	0.9826	1.0000	1.0000	0.0000
Total kg/h	3.1102	437.7448	209.0116	551.1277	79.6517	551.1277	579.0759	69.4716	5491.6862
Flowrates in kg/h									
Propylene	0.0000	0.0000	199.0611	0.0000	0.0000	0.0000	11.5034	2.6452	0.0000
Carbon Monoxide	0.0000	209.2703	0.0000	0.0000	0.0000	0.0000	211.0455	10.8989	0.0000
Hydrogen	0.0000	228.4746	0.0000	0.0000	0.0000	0.0000	244.7614	30.0626	0.0000
Propane	0.0000	0.0000	9.9505	0.0000	0.0000	0.0000	67.4399	17.2353	0.0000
Water	3.1102	0.0000	0.0000	551.1277	79.6517	551.1277	4.9959	2.9878	5491.6862
N-Butyraldehyde	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	36.2920	5.2085	0.0000
Isobutyraldehyde	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0379	0.4332	0.0000

Stream No.	10	11	12	13	14	15	16	17	18
Temp C	58.4853	104.6661	120.0027	120.0000	120.0000	90.0000	58.5000	86.2139	86.2139
Pres bar	46.9000	48.0000	49.0000	48.9000	49.0000	50.5000	46.9000	25.0000	25.0000
Enth MJ/h	-1555100.0000	-38399.0000	-4674.7000	-9.1251	-1587600.0000	1111.9000	-1554200.0000	-4167.4000	-609.0600
Vapor mass fraction	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000
Total kmol/h	5491.6862	579.0759	69.6073	0.1357	5826.2505	209.0116	5488.5762	66.9564	2.6509
Flowrates in kmol/h									
Propylene	0.0000	11.5034	2.6504	0.0052	11.6731	199.0611	0.0000	2.5906	0.0598
Carbon Monoxide	0.0000	211.0455	10.9202	0.0213	12.3391	0.0000	0.0000	10.9199	0.0004
Hydrogen	0.0000	244.7614	30.1212	0.0587	18.4528	0.0000	0.0000	30.1204	0.0008
Propane	0.0000	67.4399	17.2690	0.0337	68.5937	9.9505	0.0000	17.0412	0.2278
Water	5491.6862	4.9959	2.9936	0.0058	5493.6959	0.0000	5488.5762	2.2026	0.7910
N-Butyraldehyde	0.0000	36.2920	5.2187	0.0102	207.9012	0.0000	0.0000	3.7455	1.4732
Isobutyraldehyde	0.0000	3.0379	0.4340	0.0008	13.5945	0.0000	0.0000	0.3361	0.0979

Stream No.	19	20	21	22	23	24	25	26	27
Temp C	120.0000	54.3049	120.0000	117.9268	41.3395	23.3124	80.2069	77.8645	60.0000
Pres bar	48.9000	51.0000	48.9000	47.9000	2.0000	51.0000	50.0000	48.0000	47.0000
Enth MJ/h	-58959.0000	239.7800	-1528600.0000	-1529500.0000	-156780.0000	-454.5900	-22947.0000	-43506.0000	-44200.0000
Vapor mass fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0648
Total kmol/h	337.5383	209.0116	5488.5762	5488.5762	551.1277	209.0116	437.7448	196.2073	196.2073
Flowrates in kmol/h									
Propylene	11.6680	199.0611	0.0000	0.0000	0.0000	199.0611	0.0000	0.1646	0.1646
Carbon Monoxide	12.3178	0.0000	0.0000	0.0000	0.0000	0.0000	209.2703	10.5425	10.5425
Hydrogen	18.3942	0.0000	0.0000	0.0000	0.0000	0.0000	228.4746	2.1072	2.1072
Propane	68.5600	9.9505	0.0000	0.0000	0.0000	9.9505	0.0000	1.1201	1.1201
Water	5.1140	0.0000	5488.5762	5488.5762	551.1277	0.0000	0.0000	0.1181	0.1181
N-Butyraldehyde	207.8910	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	171.5991	171.5991
Isobutyraldehyde	13.5936	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	10.5557	10.5557

Stream No.	28	29	30	31	32	33	34	35	36
Temp C	33.0000	15.0100	29.9744	29.9744	113.4187	30.6865	48.0536	104.7090	47.9359
Pres bar	46.0000	4.0000	4.9000	4.9000	22.0000	5.0000	5.0000	4.1000	4.0000
Enth MJ/h	-45086.0000	-143.3400	-1260.3000	-43917.0000	-5571.0000	-44526.0000	-43976.0000	-2478.0000	-43980.0000
Vapor mass fraction	0.0634	1.0000	1.0000	0.0000	0.0000	0.0001	0.0001	1.0000	0.0002
Total kmol/h	196.2073	1.5533	12.9795	183.2278	81.4892	185.8787	185.8787	12.7778	185.8787
Flowrates in kmol/h									
Propylene	0.1646	0.2042	0.0116	0.1530	2.8064	0.2128	0.2128	0.2128	0.2128
Carbon Monoxide	10.5425	0.0386	10.5043	0.0382	21.4628	0.0386	0.0386	0.0386	0.0386
Hydrogen	2.1072	0.0103	2.0977	0.0095	32.2284	0.0103	0.0103	0.0103	0.0103
Propane	1.1201	1.2552	0.0691	1.0510	18.3655	1.2788	1.2788	1.2788	1.2788
Water	0.1181	0.0002	0.0160	0.1021	2.2189	0.8931	0.8931	0.8931	0.8931
N-Butyraldehyde	171.5991	0.0000	0.2567	171.3424	4.0022	172.8156	172.8156	0.0396	172.8156
Isobutyraldehyde	10.5557	0.0448	0.0241	10.5317	0.4050	10.6296	10.6296	12.4443	10.6296

Stream No.	37	38	39	40	41	42	43
Temp C	133.5177	30.0000	127.4665	111.0209	36.0000	35.1276	36.0000
Pres bar	5.0000	4.0000	2.5000	4.1000	21.5000	4.5000	3.6000
Enth MJ/h	-37782.0000	-41572.0000	-18996.0000	-2432.6000	-5979.6000	-44389.0000	-2570.1000
Vapor mass fraction	0.0000	0.0000	1.0000	0.0000	0.9177	0.0001	0.0000
Total kmol/h	173.0999	173.0999	79.6517	10.4222	81.4892	185.8787	10.4222
Flowrates in kmol/h							
Propylene	0.0000	0.0000	0.0000	0.0042	2.8064	0.2128	0.0042
Carbon Monoxide	0.0000	0.0000	0.0000	0.0000	21.4628	0.0386	0.0000
Hydrogen	0.0000	0.0000	0.0000	0.0000	32.2284	0.0103	0.0000
Propane	0.0000	0.0000	0.0000	0.0094	18.3655	1.2788	0.0094
Water	0.0000	0.0000	79.6517	0.0000	2.2189	0.8931	0.0000
N-Butyraldehyde	172.7276	172.7276	0.0000	0.0469	4.0022	172.8156	0.0469
Isobutyraldehyde	0.3723	0.3723	0.0000	10.3618	0.4050	10.6296	10.3618

Stream No.	1	2	3	4	5	6	7	8	9
Temp C	40.0000	20.0000	20.0000	20.0000	20.0000	111.3873	106.1844	120.0000	58.6217
Pres bar	48.0000	30.0000	20.0000	2.0000	3.0000	1.5000	51.0000	49.0000	51.0000
Enth MJ/h	-885.0600	-23744.0000	-525.8700	-157660.0000	-22786.0000	-132050.0000	-38253.0000	-4665.5000	-1555000.0000
Vapor mass fraction	0.0000	1.0000	0.0000	0.0000	0.0000	0.9826	1.0000	1.0000	0.0000
Total kg/h	56.0302	6322.2192	8815.4694	9928.5656	1434.9260	9928.5656	12788.6355	1697.8341	98932.7271
Flowrates in kg/h									
Propylene	0.0000	0.0000	8376.6905	0.0000	0.0000	0.0000	484.0730	111.3148	0.0000
Carbon Monoxide	0.0000	5861.6604	0.0000	0.0000	0.0000	0.0000	5911.3841	305.2793	0.0000
Hydrogen	0.0000	460.5590	0.0000	0.0000	0.0000	0.0000	493.3901	60.6001	0.0000
Propane	0.0000	0.0000	438.7790	0.0000	0.0000	0.0000	2973.8289	760.0082	0.0000
Water	56.0302	0.0000	0.0000	9928.5656	1434.9260	9928.5656	90.0010	53.8251	98932.7271
N-Butyraldehyde	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2616.9051	375.5702	0.0000
Isobutyraldehyde	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	219.0538	31.2363	0.0000

Stream No.	10	11	12	13	14	15	16	17	18
Temp C	58.4853	104.6661	120.0027	120.0000	120.0000	90.0000	58.5000	86.2139	86.2139
Pres bar	46.9000	48.0000	49.0000	48.9000	49.0000	50.5000	46.9000	25.0000	25.0000
Enth MJ/h	-1555100.0000	-38399.0000	-4674.7000	-9.1251	-1587600.0000	1111.9000	-1554200.0000	-4167.4000	-609.0600
Vapor mass fraction	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000
Total kg/h	98932.7271	12788.6355	1701.1538	3.3199	118839.0535	8815.4694	98876.6942	1561.0396	140.1143
Flowrates in kg/h									
Propylene	0.0000	484.0730	111.5325	0.2177	491.2176	8376.6905	0.0000	109.0157	2.5167
Carbon Monoxide	0.0000	5911.3841	305.8759	0.5966	345.6170	0.0000	0.0000	305.8657	0.0101
Hydrogen	0.0000	493.3901	60.7184	0.1183	37.1972	0.0000	0.0000	60.7168	0.0016
Propane	0.0000	2973.8289	761.4947	1.4865	3024.7065	438.7790	0.0000	751.4505	10.0442
Water	98932.7271	90.0010	53.9304	0.1053	98968.9294	0.0000	98876.6942	39.6801	14.2504
N-Butyraldehyde	0.0000	2616.9051	376.3046	0.7344	14991.1304	0.0000	0.0000	270.0743	106.2304
Isobutyraldehyde	0.0000	219.0538	31.2973	0.0611	980.2577	0.0000	0.0000	24.2364	7.0610

Stream No.	19	20	21	22	23	24	25	26	27
Temp C	120.0000	54.3049	120.0000	117.9268	41.3395	23.3124	80.2069	77.8645	60.0000
Pres bar	48.9000	51.0000	48.9000	47.9000	2.0000	51.0000	50.0000	48.0000	47.0000
Enth MJ/h	-58959.0000	239.7800	-1528600.0000	-1529500.0000	-156780.0000	-454.5900	-22947.0000	-43506.0000	-44200.0000
Vapor mass fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0233
Total kg/h	19959.0423	8815.4694	98876.6942	98876.6942	9928.5656	8815.4694	6322.2192	13492.6260	13492.6260
Flowrates in kg/h									
Propylene	490.9998	8376.6905	0.0000	0.0000	0.0000	8376.6905	0.0000	6.9268	6.9268
Carbon Monoxide	345.0204	0.0000	0.0000	0.0000	0.0000	0.0000	5861.6604	295.2961	295.2961
Hydrogen	37.0790	0.0000	0.0000	0.0000	0.0000	0.0000	460.5590	4.2477	4.2477
Propane	3023.2202	438.7790	0.0000	0.0000	0.0000	438.7790	0.0000	49.3913	49.3913
Water	92.1285	0.0000	98876.6942	98876.6942	9928.5656	0.0000	0.0000	2.1275	2.1275
N-Butyraldehyde	14990.3968	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	12373.4931	12373.4931
Isobutyraldehyde	980.1967	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	761.1429	761.1429

Stream No.	28	29	30	31	32	33	34	35	36
Temp C	33.0000	15.0100	29.9744	29.9744	113.4187	30.6865	48.0536	104.7090	47.9359
Pres bar	46.0000	4.0000	4.9000	4.9000	22.0000	5.0000	5.0000	4.1000	4.0000
Enth MJ/h	-45086.0000	-143.3400	-1260.3000	-43917.0000	-5571.0000	-44526.0000	-43976.0000	-2478.0000	-43980.0000
Vapor mass fraction	0.0222	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0001
Total kg/h	13492.6260	68.2769	322.5253	13170.1014	1951.8416	13310.2145	13310.2145	828.4275	13310.2145
Flowrates in kg/h									
Propylene	6.9268	8.5925	0.4877	6.4391	118.0959	8.9558	8.9558	8.9558	8.9558
Carbon Monoxide	295.2961	1.0801	294.2261	1.0699	601.1719	1.0801	1.0801	1.0801	1.0801
Hydrogen	4.2477	0.0208	4.2285	0.0192	64.9661	0.0208	0.0208	0.0208	0.0208
Propane	49.3913	55.3484	3.0475	46.3437	809.8464	56.3879	56.3879	56.3879	56.3879
Water	2.1275	0.0044	0.2881	1.8394	39.9726	16.0898	16.0898	16.0898	16.0898
N-Butyraldehyde	12373.4931	0.0019	18.5101	12354.9835	288.5863	12461.2136	12461.2136	2.3196	12461.2136
Isobutyraldehyde	761.1429	3.2290	1.7372	759.4058	29.2025	766.4667	766.4667	819.4805	766.4667

Stream No.	37	38	39	40	41	42	43
Temp C	133.5177	30.0000	127.4665	111.0209	36.0000	35.1276	36.0000
Pres bar	5.0000	4.0000	2.5000	4.1000	21.5000	4.5000	3.6000
Enth MJ/h	-37782.0000	-41572.0000	-18996.0000	-2432.6000	-5979.6000	-44389.0000	-2570.1000
Vapor mass fraction	0.0000	0.0000	1.0000	0.0000	0.8232	0.0000	0.0000
Total kg/h	12481.7165	12481.7165	1434.9260	745.6957	1951.8416	13310.2145	745.6957
Flowrates in kg/h							
Propylene	0.0000	0.0000	0.0000	0.1491	118.0959	8.9558	0.1491
Carbon Monoxide	0.0000	0.0000	0.0000	0.0000	601.1719	1.0801	0.0000
Hydrogen	0.0000	0.0000	0.0000	0.0000	64.9661	0.0208	0.0000
Propane	0.0000	0.0000	0.0000	0.4474	809.8464	56.3879	0.4474
Water	0.0000	0.0000	1434.9260	0.0000	39.9726	16.0898	0.0000
N-Butyraldehyde	12454.8704	12454.8704	0.0000	3.4302	288.5863	12461.2136	3.4302
Isobutyraldehyde	26.8464	26.8464	0.0000	741.1669	29.2025	766.4667	741.1669

Equipment Listing

The process consists of the units listed below. Unit number, function, temperature and pressure level are stated in the table below.

Unit number	Description	Operating P (bar)	Operating T (°C)
R1 (a,b and c)	Hydroformylation reactor	50.0	120[10]
C1	Syn gas/recycle compressor	49.5[2]	105
C2	Syn gas feed compressor	40.0	60
E1	Reactor section off gas expander	37.0[3]	104
E2	Settler off gas expander	25.0	32
GLS1	N/I column reflux drum	4.1	105
GLS2	I/lights column reflux drum	4.0	15
H1[1]	water recycle/ propylene feed	48.0[4]	70
H2	water recycle/cooling water	46.2	40
H3	product/propylene feed	51.0	30
H4	product/cooling water	46.5	41
H5	N/I column reboiler	5.0[5]	50
H6	N/I column reflux condensor	5.0	50
H7	n-butyraldehyde/cooling water	4.5	80
H8	I/lights column reboiler	4.1	105
H9	I/lights condensor	4.1	105
H10	fuel gas/product	4.3	42
H11	I-butyraldehyde/product	3.8	74
P1	water recycle pump	49.0[6]	58
P2	propylene feed pump	38.0	21
P3	vessel effluent pump	4.5	49
S1	three phase settler	49.0[7]	120
T1	stripper	48.9[8]	120
T2	N/I separation column	5.0	50
T3	I/lights separation column	4.1	105
V1	Buffer vessel	4.9[9]	30

[1] All units that are listed as H# are heat exchangers

[2] The mean pressure of the feed and the effluent stream of the compressor is chosen as the operating pressure

[3] The mean pressure of the feed and the effluent stream of the expander is chosen as the operating pressure

(4 The mean pressure of the feed and the effluent stream of the heat exchanger is chosen as the operating pressure; The pressure is based on the product stream going through the heat exchanger.

(5 All heat exchangers on distillation columns are chosen to be operated at the column feed pressure

(6 The mean pressure of the feed and the effluent stream of the pump is chosen as the operating pressure

(7 The operating pressure of the settler is the feed pressure

(8 The operating pressure of the distillation columns is the feed pressure

(9 The operating pressure of the buffer vessel is the feed pressure

(10 All the same rules hold for the operating temperatures as for the operating pressures

Appendix 7
Process Economics

Appendix 7A

Production costs calculations

material & financial balance

Feed	Amount (ton/a)	Products	Amount (ton/a)
propylene	71087.90	n-butyraldehyde	100654.10
syngas	50982.40	i-butyraldehyde	6012.20
water (cooling)	2444524.25	fuel gas	1739.70
water (process)	451.80	steam (2.5 bar)	11571.40
catalyst	0.046375	steam (1.5 bar)	80064.00
Sum	214157.50		214041.4**

* rhodium and ligand losses are neglected.

** n-/i-Butyraldehyde distillation uses a waterdecant of 116.1 ton/a.

	prices ($)		consumption ($/a)
raw materials:			
propylene	271.20	/ton	19279038.48
syngas	4.40	/ton	224187.07
water (process)	1.56	/ton	705.94
water (cooling)	0.06	/ton	152782.77
catalyst	218063.93	/ton	10112.71
utilities:			
electricity:	0.05	/kWh	119616.75
steam	0.01	/kWh	2832224.64
products:			
n-butyraldehyde	677.70	/ton	-68213283.57
i-butyraldehyde	703.30	/ton	-4228380.26
fuel gas	1.50	/ton	-2609.55
steam (1.5bar)	18.75	/ton	-1501200.00
steam (2.5 bar)	18.75	/ton	-216963.75

Total proceeds: **74162437.13** $/a

Total consumption: **-51543768.76** $/a

total production costs

Production volume dependent costs	2.26E+07	($/a)

$K'_L = d * L$

$L = 20 * N * C^{.24}$

d	2.60	(-)	
N	4.00	(-)	(N=4: compression-, reaction-,
C	214.00	(kton/a)	decompression- and
L	289994.19	($/a)	separation-section)
K'_L	753984.89	($/a)	

labour dependent costs	7.54E+05	($/a)

$K'_l = f * l$

f 0.233 (-)

	Taylor	Miller	Zev-Buch.	
l	87334514.688	81313333.3333	77892069.548855	($/a)
K'_l	20348941.922304	18946006.6667	18148852.204883	($/a)

Investment dep. costs	2.03E+07	1.89E+07	1.81E+07	($/a)

$K_t = a * K_p + K'_L + K'_l$

a 1.13 (-)

	Taylor	Miller	Zev-Buch.	
K_t	46662022.0630266	45259086.8074	44461932.345606	($/a)

Total prod. costs	4.67E+07	4.53E+07	4.45E+07	($/a)

total anual profit

Profit is defined as:

Profit = Proceeds - Production Costs

	Taylor	Miller	Zev-Buch.	
Profit	**2.75E+07**	**2.89E+07**	**2.970E+07**	**($/a)**

Calculations:

Prices:					
Rh	43400000	$/ton			
Tppts	61062.5	$/ton	molm.	574 kg/kmol	
Consumption:					
Rh	0.000168	ton/a		7291.2	$/a
TPPTS	0.046207	ton/a		2821.515	$/a
SUM	**0.046375**	**ton/a**		**10112.71**	**$/a**

energy requirement		
equipment	power kW	
13	40.7434	
19	11.46	
reactor	44.7	
21	221.4483	
8	12.46	
14	-28.2809	
expander	-25.5611	
11	22.69	
SUM	299.6597	kW
Total	**2416500**	**kWh/a**

cooling water requirement			
Q	18180000	7.6E+04	kJ/h
T-heat	15	10	°C
Heat capacity	4.18	4.18	kJ/kg K
Flow	289952.2	1824.738	kg/h
	2338174	**14714.69**	**ton/a**
Total	**2352889**		**ton/a**

steam requirement		
Price	0.006756	$/kWh
Flow	4.19E+08	kWh/a
consumption	**2832225**	**$/a**

Appendix 7B **Investments** *Taylor*

	massflow [kg/h]	rel.throughput [t/t product]	rel.throughput [score]	construction material	construction material [score]	reaction/storage [score]
Storage/Handling						
propylene (feed)	8376.7	11.4	-1.0	SS	1	1
propane (feed)	438.78	0.0	-4.0	SS	1	1
syngas (feed)	6355.2	8.6	-1.5	SS	1	1
water (feed1)	56.0	0.1	-4.0	SS	1	1
water (feed2)	9928.6	13.5	-0.5	SS	1	1
water (feed3)	1435.0	1.9	-3.5	SS	1	1
water (recycle)	98876.7	134.3	4.0	SS	1	1
n-butyraldehyde	12455.1	16.9	0.0	SS	1	1
i-butyraldehyde	736.4	1.0	-4.0	SS	1	1
purge	1951.8	2.7	-3.5	SS	1	1
steam	9928.6	13.5	-0.5	SS	1	1
steam	1435.0	1.9	-3.5	SS	1	1
Processes						
reactor (1) [3X]	40178.9	54.6	1.0	SS	1	0
expander (3)	118839.0	161.4	4.0	SS	1	0
stripper (5)	26281.3	35.7	1.0	SS	1	0
dist.column (10)	13310.2	18.1	0.0	SS	1	0
dist.column (16)	828.3	1.1	-4.0	SS	1	0

	P [bar]	P [score]	T [degr C]	T [score]	total score	costliness index
Storage/Handling						
propylene (feed)	20.0	1.5	20.0	0.0	2.5	2.0
propane (feed)	20.0	1.5	20.0	0.0	-0.5	0.9
syngas (feed)	30.0	1.5	20.0	0.0	2.0	1.7
water (feed1)	48.0	2.0	40.0	0.0	0.0	1.0
water (feed2)	2.5	0.5	20.0	0.0	2.0	1.7
water (feed3)	3.0	0.5	20.0	0.0	-1.0	0.8
water (recycle)	48.9	2.0	120.0	0.5	8.5	8.9
n-butyraldehyde	4.0	0.5	30.0	0.0	2.5	2.0
i-butyraldehyde	3.6	0.5	36.0	0.0	-1.5	0.7
purge	21.5	1.5	36.0	0.0	0.0	1.0
steam	1.5	0.5	111.4	0.5	2.5	2.0
steam	2.5	0.5	127.5	0.5	-0.5	0.9
Processes						
reactor (1) [3 X]	50.0	2.0	120.0	0.5	4.5	3.2
expander (3)	49.0	2.0	120.0	0.5	7.5	7.2
stripper (5)	49.5	2.0	100.0	0.5	4.5	3.3
dist.column (10)	5.0	1.0	48.0	0.0	2.0	1.7
dist.column (16)	4.1	0.5	104.7	0.5	-2.0	0.8
				total	**42.0**	**46.2**

Appendix 7B. Miller's Method

Miller's method of calculating I_F employed various prices. This appendix aims to clarify two main aspects:

1. How prices were calculated and
2. Why a particular percentage was chosen when prices had to be selected from a given range.

Explanations pertaining to PI_{1995}

This section is sub-divided into two sections. The first is concerned with the unit costs of the PI, the second with the actual PI_{1995}.

Calculations of unit costs in the PI

- Currency values:

US Dollar value and British Pound value were obtained from the NOS teletext financial pages. One US dolar represents hfl 1.698, one British pound represents hfl 2.688, the date is 14-11-1996.

- Reactors

The process uses four reactors with a 40 m^3 capacity (S). Reactor conditions can be set at 120 ° C and 50 bar. The reactor costs are determined using table 6.2 and equation 6.7 (Coulson and Richardson,1991). Table 6.2 gives values for C (£ 8000) and index n (0.40) for jacketed reactors made of carbon steel. The purchased equipment cost per reactor can now be calculated with the following equation

$$Ce = CS^n$$

where Ce = purchased equipment cost ($)
S = caracteristic size parameter
C = cost constant ($)
n = equipment type index

The purchased equipment cost for an individual reactor is 55,979.2 $. If the reactor is seen as a stainless steel constructed pressure vessel the equipment costs can be calculated from fig 6.4 (Coulson and Richardson).

Diameter (m)	Height (m)	Material factors	Pressure factors	Equipment Cost ($)
2.94	5.88	S.S. ×2	40-50 bar ×1.8	80,640

This means that the total reactor costs equal 322,560 $.

- Columns

The process uses two distillation columns and a stripper.

N/I-separation Dist.Column	D(m)	H(m)	Average wall thickness (mm)	Material	Equipment costs ($)
rectifying section	1.57	18.04	14.00	Steel H II	289,000
stripping section	1.77	28.72	18.00	Steel H II	622,200

I/lights sep. Dist.Column	**D(m)**	**H(m)**	**Average wall thickness (mm)**	**Material**	**Equipment costs ($)**
rectifying section	0.24	6.00	8.00	Steel H II	85,000
stripping section	0.13	2.00	8.00	Steel H II	85,000

Stripper	**D(m)**	**H(m)**	**Average wall thickness (mm)**	**Material**	**Equipment costs ($)**
total section	0.64	7.22	8.00	Steel H II	85,000

Process	**Internals**	**D_{int} (m) rect.sec.**	**D_{int} (m) strip.sec.**	**Type**	**Costs ($)**
N/I-sep.	sieve tray	1.83	2.13	AISI 405	589,630
I/Purge-sep.	sieve tray	0.31	0.15	AISI 405	27,800
Stripper	sieve tray	0.91	0.76	AISI 405	206,069

Process	**Packings**	**D (mm)**	**Type**	**Costs ($)**
N/I-sep.	Raschig rings	16	C.S.	702,304
I/Purge-sep.	Raschig rings	16	C.S.	2,291
Stripper	Raschig rings	16	C.S.	18,773

All prices are obtained from DACE prijzenboekje (1994).

- Heat exchangers.

The total of heat exchangers in the process adds up to ten. All heat exchangers contain bundle of pipes for heat exchange and are made of stainless steel (AISI 304).

unit	**A (m^2)**	**Material**	**costs ($)**
H2	312	AISI 304	505,648
H7	131	AISI 304	314,007
H3	21	AISI 304	78,540
H4	14	AISI 304	65,054
H1	6	AISI 304	57,375
H11	5	AISI 304	57,375
H10	25	AISI 304	93,500
H5	77	AISI 304	102,000

unit	A (m^2)	Material	costs ($)
H6	101	AISI 304	141,000
H8	56	AISI 304	416,000
H9	2	AISI	57,375

- Pumps

The process contains three one step centrifugal pumps, that are made of stainless steel.

unit	Capacity (m^3/h)	Max.P. needed (kW)	Material	Pump costs ($)	Electro engine	E-engine costs ($)	total costs ($)
P1	17.33	19.90	AISI 316	20,400	'EX'E	7,140	27,540
P2	100.58	22.35	AISI 316	21,080	'EX'N	5,610	26,690
P3	16.63	0.62	AISI 316	14,280	'EX'E	629	14,909

All pumps are supplied without electro engines, which have to be purchased separately.

- Compressors

The process uses two centrifugal compressors. The costs can be calculated using table 6.2 and equation 6.7 (Coulson and Richardson, 1991)

unit	Driver Power (kW)	Constant C (£)	Index n	costs ($)
C1	82.97	500	0.8	10,714
C2	467.39	500	0.8	42,716

- Expanders

The process uses two turbine expanders. The costs can be calculated using table 6.2 and equation 6.7 (Coulson and Richardson, 1991)

unit	Driver Power (kW)	Constant C (£)	Index n	costs ($)
E1	79.24	3200	0.5	17,803
E2	93.09	3200	0.5	19,296

- Reflux drums

The reflux drums are taken as horizontal tanks, the construction material is carbon steel.

	Size S (m^3)	Constant C (£)	index n	costs ($)
N/I separator column	45	1250	0.60	19,632
I/Fuel gas separator column	1.1	1250	0.60	2,118

- Buffer vessel

The buffer vessel is taken as a vertical tank, the construction material is carbon steel.

	Size S (m^3)	**Constant C (£)**	**index n**	**costs (\$)**
Vessel (V1)	8	1250	0.60	7,400

- Settler

The settler is taken as a horizontal vessel, the construction material is carbon steel.

	Size S (m^3)	**Constant C (£)**	**index n**	**costs (\$)**
Settler (S1)	90	1500	0.60	146,338

Appendix 7D **Investments** *Zevnik-Buchanon*

Functional Units	Tmax (°K)	F_t	P max(bar)	F_p	Material	F_m
reactor (1)	393.150	0.019	50.000	0.170	SS	0.100
settler (3)	393.150	0.019	49.900	0.170	SS	0.100
stripper (5)	373.150	0.015	50.000	0.170	SS	0.100
dist.column (10)	406.150	0.021	5.000	0.070	SS	0.100
dist.column (16)	403.150	0.020	4.100	0.061	SS	0.100

Functional Units	C_f	pi (kton/a)	Ie (M$)	Cf*pi^m	Ib (k$)	It (k$)
reactor (1)	3.886	324.003	1.300	374.063	58419.05	77892.07
settler (3)	3.885	958.318	1.300	238.953		
stripper (5)	3.854	211.932	1.300	95.854		
dist.column (10)	3.103	107.334	0.900	51.319		
dist.column (16)	3.039	6.679	0.900	9.495		

Ib (M$)	It (M$)
58.42	77.89

$It = Ib / 0.75$ (PEP YEARBOOK)

Calculations

Functional Units	Pi (kg/h)	Pi (ton/a)
reactor (1)	120536.8	972.009
settler (3)	118839.0	958.318
stripper (5)	26281.3	211.932
dist.column (10)	13310.2	107.334
dist.column (16)	828.3	6.679

Economical Criteria

Static methods

ROI : *Return On Investments.*

Data:

Taylor		
W_a	2.8E+07	($)
I_F	6.6E+07	($)
I_W	5.2E+06	($)
Miller		
W_a	2.9E+07	($)
I_F	6.1E+07	($)
I_W	4.9E+06	($)
Zevn.-Buch.		
W_a	3.0E+07	($)
I_F	5.84E+07	($)
I_W	4.7E+06	($)

Taylor

*I_W = 0.06 * I_T*

*I_F = 0.75 * I_T*

I_T	87334515	($)
I_W	5.2E+06	($)

ROI:

Taylor	39	(%)
Miller	44	(%)
Zev.-buch.	47	(%)

POT: *Pay-Out Time*

Data:

E_o	5.08E+07	($/a)
P	7.42E+07	($/a)
K_V	2.3E+07	($/a)

Taylor		
K_SV	7.5E+05	($/a)
I_F	6.6E+07	($)
Miller		
K_SV	7.5E+05	($/a)
I_F	6.1E+07	($)
Zev.-Buch.		
K_SV	7.5E+05	($/a)
I_F	5.84E+07	($)

POT

Taylor	1.29	(a)
Miller	1.20	(a)
Zev.-Buch.	1.15	(a)

POT [s and I_W included]

Taylor	1.52	(a)
Miller	1.43	(a)
Zev.-Buch.	1.38	(a)

Dynamic methods

IRR: *Internal Rate of Return*

Cashflow = Proceeds - Productcosts - Depreciation.
*Depreciation = 0.08 * I_F*

Taylor

I_F	6.55E+07	($)
s	6550089	($)
I_W	5240071	($)

Year	Cashflow
0	-7.2E+07
1-14	2.23E+07
15	3.41E+07

	N.C.F.	D.C.F.
in	7.21E+07	7.21E+07
out	3.46E+08	5.52E+07
RATIO	4.797927	0.765431

Ratio calculation (D.C.F.)	
i(II)	0.4
out (i(II))	5.5E+07

IRR Calculation	
i	0.304124
Sum =	-6.2E-09

IRR: **30.412** (%)

Miller

I_F	6.1E+07	($)
s	6098500	($)
I_W	4878800	($)

Year	Cashflow
0	-6.7E+07
1-14	2.4E+07
15	9.61E+07

	N.C.F.	D.C.F.
in	6.71E+07	6.71E+07
out	4.32E+08	5.95E+07
RATIO	6.445985	0.887265

Ratio calculation (D.C.F.)	
i(II)	0.4
out (i(II))	6.0E+07

IRR Calculation	
i	0.3584
Sum =	-3.2E-07

IRR: **35.840** (%)

Zev.-Buch.

I_F	5.84E+07	($)
s	5841905	($)
I_W	4673524	($)

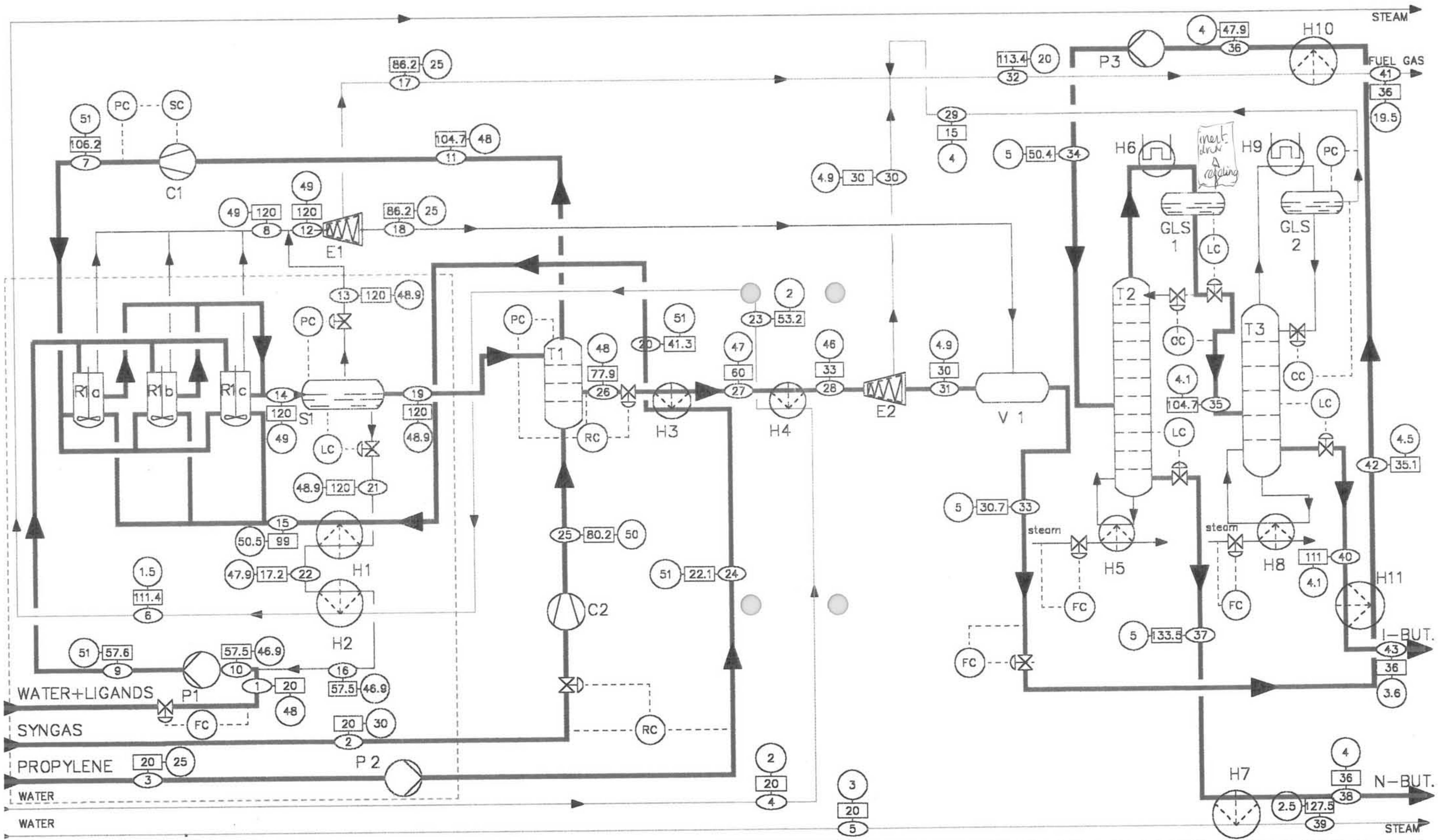
Year	Cashflow
0	-6.4E+07
1-14	2.5E+07
15	9.21E+07

	N.C.F.	D.C.F.
in	6.43E+07	6.43E+07
out	4.42E+08	6.2E+07
RATIO	6.885802	0.964884

Ratio calculation (D.C.F.)	
i(II)	0.4
out (i(II))	6.2E+07

IRR Calculation	
i	0.389582
Sum =	-7.3E-07

IRR: **38.958** (%)



C1	SYNGAS COMPRESSOR	GLS2	GAS-LIQUID SEPARATOR	H5	REBOILER	H10	HTXR:FUEL GAS-PRODUCT	R1a	CSTR WITH GAS INLET	T2	N/I-DIST. COLUMN
C2	SYNGAS COMPRESSOR	H1	HTXR:WATER REC.-PROPYLENE	H6	CONDENSOR	H11	HTXR:I-BUT.-PRODUCT	R1b	CSTR WITH GAS INLET	T3	I/LIGHTS-DIST. COLUMN
E1	EXPANDER	H2	HTXR:WATER REC.-WATER	H7	HTXR:N-BUT.-WATER	P1	PUMP	R1c	CSTR WITH GAS INLET	V1	VESSEL
E2	EXPANDER	H3	HTXR:PRODUCT-PROPYLENE	H8	REBOILER	P2	PUMP	S1	3-PHASE SETTLER		
GLS1	GAS-LIQUID SEPARATOR	H4	HTXR:PRODUCT-WATER	H9	CONDENSOR	P3	PUMP	T1	STRIPPER		

PROCESS FLOWSHEET FOR THE PRODUCTION OF N/I-BUTYRALDEHYDE

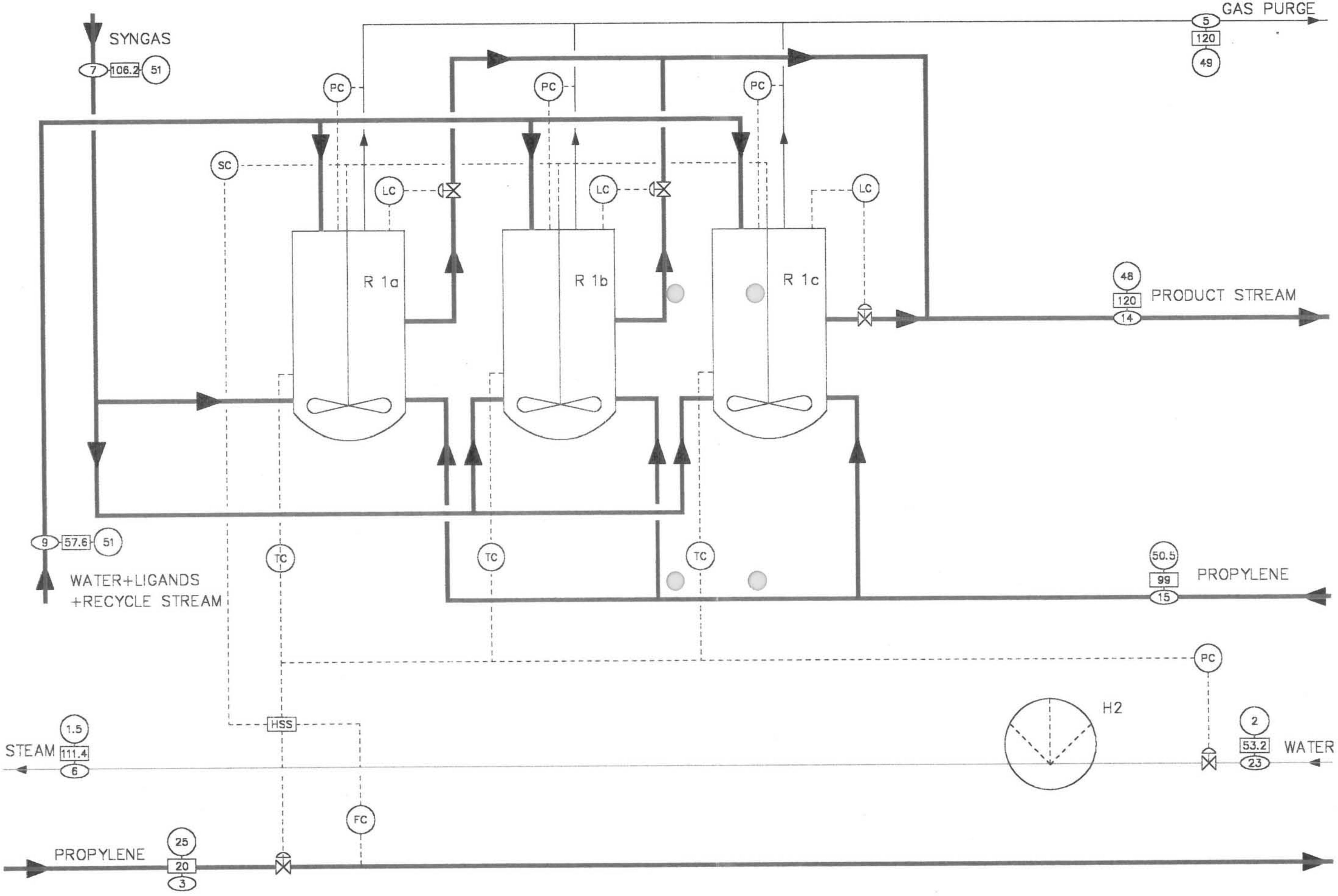
FVO 3188 **SEPTEMBER 1996**

MAIN STREAM
FUEL GAS
WATER RECYCLE
WATER/STEAM
ZOOM IN FOR PROCESS CONTROL

streamnr. (nr.)
pressure (bar) (P)
temperature (C) T

E.V.Verhoef
C.A.A.Schuurmans
R.M.Lenz
G.A.Pouw

ZOOM IN ON REACTOR SYSTEM FOR PROCESS CONTROL



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