Aspen Tutorials

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Preface

The research in Plant Design focuses on a process feasibility study, synthesis, design, operation, integration, simulation and optimization, inherent safety, occupational health, pollution prevention and industrial risk. The key theme is the development of systematic methodologies to identify optimum, sustainable and creative strategies that lead to process intensification, yield improvement, debottlenecking, costing, safety, pollution prevention and energy conservation. Fundamental chemical engineering principles are coupled with systems engineering approaches to develop methods and computer-aided tools applicable in all chemical process industry areas. Any plant design work includes preliminary process design, process synthesis, cost engineering, process simulation and environmental and safety aspects of design. This knowledge can be used for developing new processes, engineering new plants and improving existing ones in the chemical, petrochemical, biofuel, pulp and paper, minerals, food and biotech and pharmaceutical industries.

These lecture notes are a collection of simulations the Plant Design group uses while teaching master students.

Contents

Chapter 1

Thermochemical processes

1.1 Production of synthetic gas from a biomass

The task is to simulate the production of synthetic gas from biomass. One way to do it is to develop an Aspen model. The model is divided into the biomass decomposition, gasification and separation units where the solids and syngas are separated. In the simulation, the gasifier is in an isothermal steady state. Decomposition products are estimated based on the ultimate biomass analysis. The model does not consider tars, but ashes are described as non-conventional solids. Biomass is pine sawdust, which is a common waste product of the forest industry. Figure 1.1 presents the process flow diagram.
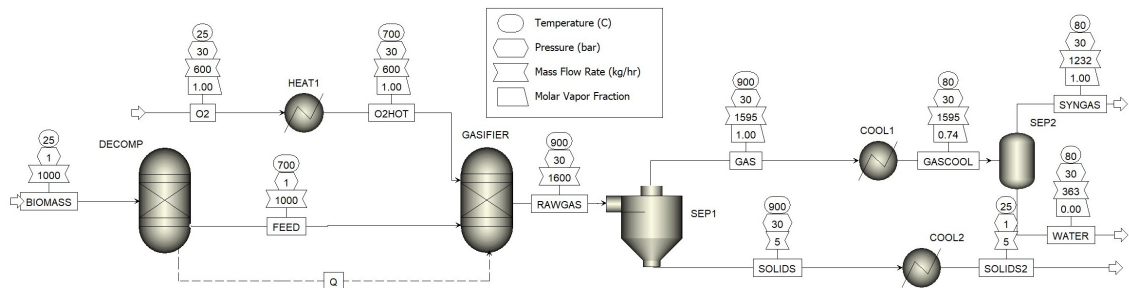

Figure 1.1: Gasification production plant

Add all simulation's components can be found in the table 1.1.

The next step is to select a thermodynamic model. The chosen property method is the Redlich-Kwong-Soave cubic equation of state with Boston-Mathias alpha function ($RKS - BM$). This method is suitable for non-polar or slightly polar mixtures like hydrocarbons and light gases. The database of Aspen contains only conventional components, which means that the properties of the biomass and the coal needs to be specified manually. In the software, the properties of the non-conventional components can be specified in the "Method/NC Props" tab. HCOALGEN and DCOALIGT models can estimate biomass and ash properties. HCOALGEN and DCOALIGT models are used to calculate the enthalpy and density of non-conventional components, respectively. The HCOALGEN model requires these three component attributes for non-conventional components: proximate analysis results (denoted as PROXANAL in Aspen Plus), ultimate analysis results (denoted

Component ID	Type	Coponent name	Alias
BIOMASS	Nonconventional		
ASH	Nonconventional		
H_2	Conventional	HYDROGEN	H_2
O_2	Conventional	OXYGEN	O_2
N_2	Conventional	NITROGEN	N_2
CO	Conventional	CARBON-MONOXIDE	CO
CO_2	Conventional	CARBON-DIOXIDE	CO_2
METHA-01	Conventional	METHANE	CH_4
CARBOGRA	Solid	CARBON-GRAPHITE	C
S	Conventional	SULFUR	S
H_2S	Conventional	HYDROGEN-SULFIDE	H_2S
H_3N	Conventional	AMMONIA	H_3N

Table 1.1: Simulation component

as ULTANAL in Aspen Plus), and sulfur analysis results (denoted as SULFANAL in Aspen Plus). The proximate analysis gives moisture, fixed carbon, volatile matter and ash weight content. The ultimate analysis gives the weight composition of coal in terms of ash, carbon, hydrogen, nitrogen, chlorine, sulfur, and oxygen. The sulfur analysis divides the sulfur content into pyritic, sulfate, and organic sulfur. The DCOALIGT model requires only the two-component attributes ULTANAL and SULFANAL. In Aspen Plus, multiple correlations have been predefined to calculate the enthalpy. The HCOALGEN option codes are shown in table 1.2.

Option Code Value	Calculation Method Parameter	Names Component	Attributes
1 - Heat of Combustion			
1	Boie correlation	BOIEC	ULTANAL/SULFANAL/PROXANAL
2	Dulong correlation	DLNGC	ULTANAL/SULFANAL/PROXANAL
3	Grummel and Davis correlation	GMLDC	ULTANAL/SULFANAL/PROXANAL
4	Mott and Spooner correlation	MTSPC	ULTANAL/SULFANAL/PROXANAL
5	IGT correlation	CIGTC	ULTANAL/PROXANAL
6	User input value	HCOMB	ULTANAL/PROXANAL
2 - Standard Heat of Formation			
1	Heat-of-combusion based correlation	-	ULTANAL/SULFANAL
2	Direct correlation	HFC	ULTANAL/SULFANAL/PROXANAL
3 - Heat Capacity			
1	Kirov correlation	CP1C	PROXANAL
2	Cubic temperature equation	CP2C	-
4 - Enthalpy Basis			
1	Elements at 298.15K and 1 atm	-	-
2	Component at 298.15 K	-	-

Table 1.2: HCOALGEN Option Codes

Default = 1 for each option code. In the exercise, the HCOALGEN codes for the ash are [1 1 1 1], which means default values. In biomass, the codes [6 1 1 1] mean that the heat of combustion will be specified. The heat of combustion can be introduced by implementing a new non-conventional parameter in the "Pure Components" section. Choose the biomass from the list and select the HCMOB option to introduce a $18.4[MJ/kg]$ value.

As multiple parameters need to be evaluated, select the option "Estimate all missing parameters" from the "Estimation" tab.

Each simulation starts by defining an inlet stream. Specify the biomass feed to

be 1000[kg/h] at 25°C] and 1[bar]. Enter its Component attribute in table 1.1. Add proximate, ultimate and sulphur analysis data of biomass feed in NC Solid.

Group	Components	w-%
Moisture content	H_2O	8
Proximate analysis		
	Volatile matter (VM)	82.29
	Fixed carbon (FC)	17.16
	Ash	0.55
Ultimate analysis		
	C	50.54
	H	7.08
	O	41.11
	N	0.15
	S	0.57
	Ash	0.55
Sulfur analysis		
	Pyritic	0
	Sulfate	0.057
	Organic	0.513

Table 1.3: Characteristics of Biomass (pine sawdust)

The biomass is defined as a non-conventional solid in Aspen Plus and the ash present in the biomass. The presence of non-conventional components in the simulation needs the stream class MIXINC, which is for models where both conventional solids (carbon) and non-conventional solids are present and when particle size distribution is unknown (go to Simulation-> set up-> specification-> Global setting stream class).

When the simulation parameters are defined, the operational blocks can be introduced. The first operational unit is the decomposer. The solid biomass is decomposed at into gaseous products, which can follow further processing. For the decomposition of biomass, the DECOMP module is Aspen *RYield* reactor where the biomass is decomposed into H_2, O_2, N_2, H_2O, S, C and ash according to the biomass ultimate analysis data at 700[°C] and 1[bar]. The RYield decomposes the biomass into the constituents shown in table 1.4.

Component	Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur	Ash	Water
Yield (in mass %)	0.464968	0.065138	0.3782	0.00138	0.005244	0.00507	0.08

Table 1.4: Yields for the RYIELD reactor

The next operation unit is the gasifier (presented in figure 1.2). For that purpose, let's use the Gibbs Reactor will produce an outlet in which the Gibbs free energy of the mixture is minimised. A set of reactions can be suggested in the reactor model. However, it is important to note that the suggested reaction might not be included in the simulation as free energy minimisation will be the dominant method. An exception to this rule is the stoichiometry of the reaction set. Without

a set, stoichiometry will not be considered in the simulation; however, with an attached reaction set with stoichiometric parameters, the simulation will account for them, and the outlet conditions can change. However, if a set is attached, only the components specified in the set will reach an equilibrium point; other components will be neglected. The Gibbs Reactor can be very useful if the user does not possess any data pertinent to the reaction or desires only a simulation of the equilibrium state. At the very least, the Gibbs Reactor can provide simulation estimates as a starting point for a more rigorous simulation through another reactor type.

The pressure is at $30[bar]$ and $900[°C]$, which is a typical value for real-world gasifiers. Oxygen $600[kg/h]$ is used as the oxidising agent, which is preheated to $700[°C]$. The possible products of the gasification were predefined to be: H_2, O_2, N_2, H_2O, S, $C(solid)$, CO, CO_2, H_2S, CH_4, C and NH_3. Aspen calculated the product distributions at various conditions.

Finally, in the simulation's separation section, the solids are separated from the hot gases in SEP1, which is an Aspen SSplit. The SSPLIT assumes perfect separation of solid particles from the mainstream. The SEP2 column is a flash column used to separate the condensate. The gases are cooled to $80[°C]$ with heat exchanger COOL1. The product of the process

Figure 1.2: The gasifier

is the stream SYNGAS, which contains the main syngas components CO and H_2, but also contains impurities such as H_2S and NH_3. The product of this process needs to be further purified in a separate purification facility to be helpful feedstock for other processes.

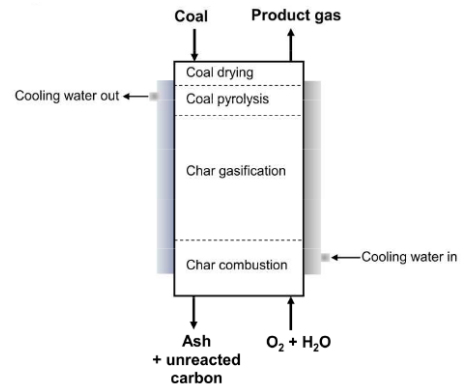The configuration of the simulation and its results are presented below:

	Units	BIOMASS	FEED	GAS	GASCOOL	O2	O2HOT	RAWGAS	SOLIDS	SOLIDS2	SYNGAS	WATER
Description												
From			DECOMP	SEP1	COOL1		HEAT1	GASIFIER	SEP1	COOL2	SEP2	SEP2
To		DECOMP	GASIFIER	COOL1	SEP2	HEAT1	GASIFIER	SEP1	COOL2			
Stream Class		MIXCINC	MIXCINC	MIXCINC	MIXCINC	MIXCINC	MIXCINC	MIXCINC	MIXCINC	MIXCINC	MIXCINC	MIXCINC
Maximum Relative Error												
Cost Flow	$/hr											
− **Total Stream**												
Temperature	C	25	700	900	80	25	700	900	900	25	80	80
Pressure	bar	1.01325	1.01325	30	30.3975	30	30	30	30	1.01325	30.3975	30.3975
Mass Vapor Fraction		0	0.529962	1	0.772277	1	1	0.996831	0	0	1	0
Mass Liquid Fraction		0	0	0	0.227723	0	0	0	0	0	0	1
Mass Solid Fraction		1	0.470038	0	1.71182e-07	0	0	0.00316875	1	1	0	0
Mass Enthalpy	kcal/kg	-2116.59	118.101	-1265.87	-1721.12	-1.84382	162.869	-1261.79	22.2112	-191.945	-1136.33	-3704.33
Mass Density	kg/cum	1209.43	0.256624	6.40179	28.9242	39.1882	11.7698	6.4221	3486.88	3486.88	22.5431	722.435
Enthalpy Flow	Gcal/hr	-2.11659	0.118101	-2.01898	-2.74507	-0.00110629	0.0977213	-2.01887	0.000112611	-0.000973161	-1.39965	-1.34542
+ **Mass Flows**	**kg/hr**	**1000**	**1000**	**1594.93**	**1594.93**	**600**	**600**	**1600**	**5.07**	**5.07**	**1231.73**	**363.202**
+ **Mass Fractions**												
Volume Flow	cum/hr	0.826835	3896.75	249.138	55.1417	15.3107	50.978	249.139	0.00145402	0.00145402	54.6389	0.502747
− **MIXED Substream**												
Phase			Vapor Phase	Vapor Phase		Vapor Phase	Vapor Phase	Vapor Phase			Vapor Phase	Liquid Phase
Temperature	C		700	900	80	25	700	900			80	80
Pressure	bar	1.01325	1.01325	30	30.3975	30	30	30		1.01325	30.3975	30.3975
Molar Vapor Fraction			1	1	0.736558	1	1	1			1	0
Molar Liquid Fraction			0	0	0.263442	0	0	0			0	1
Molar Solid Fraction			0	0	0	0	0	0			0	0
Mass Vapor Fraction			1	1	0.772277	1	1	1			1	0
Mass Liquid Fraction			0	0	0.227723	0	0	0			0	1
Mass Solid Fraction			0	0	0	0	0	0			0	0
Molar Enthalpy	kcal/mol		-0.0754248	-26.5249	-36.0642	-0.0590001	5.21161	-26.5249			-24.9653	-67.0958
Mass Enthalpy	kcal/kg		-6.94315	-1265.87	-1721.12	-1.84382	162.869	-1265.87			-1136.33	-3704.33
Molar Entropy	cal/mol-K		9.4715	13.3201	-3.0995	-6.90086	2.21927	13.3201			9.02204	-36.9901
Mass Entropy	cal/gm-K		0.871889	0.635689	-0.14792	-0.21566	0.0693548	0.635689			0.410652	-2.04221
Molar Density	kmol/cum		0.0125201	0.305518	1.38038	1.22468	0.36782	0.305518			1.02608	39.8853
Mass Density	kg/cum		0.136008	6.40179	28.9242	39.1882	11.7698	6.40179			22.5431	722.435
Enthalpy Flow	Gcal/hr		-0.00367961	-2.01898	-2.74507	-0.00110629	0.0977213	-2.01898			-1.39965	-1.34542
Average MW			10.8632	20.9539	20.9539	31.9988	31.9988	20.9539			21.97	18.1128
+ **Mole Flows**	**kmol/hr**	**0**	**48.7851**	**76.1162**	**76.1162**	**18.7507**	**18.7507**	**76.1162**	**0**	**0**	**56.064**	**20.0522**
+ **Mole Fractions**												
+ **Mass Flows**	**kg/hr**		**529.962**	**1594.93**	**1594.93**	**600**	**600**	**1594.93**			**1231.73**	**363.202**
+ **Mass Fractions**												
Volume Flow	cum/hr		3896.54	249.138	55.1417	15.3107	50.978	249.138			54.6389	0.502747
+ **Vapor Phase**												
+ **Liquid Phase**												
+ **CISOLID Substream**												
− **NC Substream**												
Temperature	C	25	700					900	900	25		
Pressure	bar	1.01325	1.01325		30.3975	30	30	30	30	1.01325	30.3975	30.3975
Mass Enthalpy	kcal/kg	-2116.59	-36.1888					22.2112	22.2112	-191.945		
Mass Density	kg/cum	1209.43	3486.88					3486.88	3486.88	3486.88		
Enthalpy Flow	Gcal/hr	-2.11659	-0.000183477					0.000112611	0.000112611	-0.000973161		
+ **Mass Flows**	**kg/hr**	**1000**	**5.07**	**0**	**0**	**0**	**0**	**5.07**	**5.07**	**5.07**	**0**	**0**
+ **Mass Fractions**												
Volume Flow	cum/hr	0.826835	0.00145402					0.00145402	0.00145402	0.00145402		

Figure 1.3: Gasification results

1.2 The fast pyrolysis of the biomass

Biomass fast pyrolysis is a highly non-equilibrium reaction where the main components (lignin, celluloses and hemicelluloses) are broken down into shorter molecules like acids, aldehydes, phenols, sugars and non-condensable gases. More than 200 different components have been identified in pyrolysis oil, and their share depends on the feedstock, process parameters and measurement equipment. Therefore, modelling biomass fast pyrolysis is not trivial. However, the following assumptions will allow the modelling of biomass fast pyrolysis:

- Biomass, ash, char, and lignin are defined as non-conventional components (neither molecular weight nor molecular structure can be given); Biomass attributes are computed with AspenPlus' built-in enthalpy and density models HCOALGEN and DCOALLIGT (for reference check chapter **??**)

- Pyrolysis is modelled with a yield reactor where the user defines the pyrolysis products.

Figure 1.4 presents the process flow diagram. The biomass is fed directly to the pyrolysis unit, which operates at high temperature and atmospheric pressure. Then the gaseous streams are cooled down, and the two-phase mixture is separated.
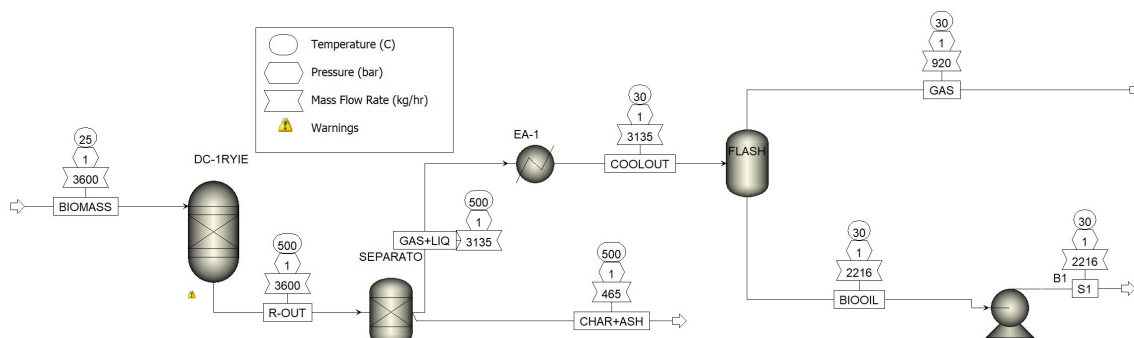

Figure 1.4: Fast pyrolysis plant

Add all the conventional components in the component list as given in the table 1.5 and non-conventional components BIOMASS, ASH, CHAR and LIGNIN.

The thermodynamic method used in this exercise is UNIQUAC (universal quasichemical), an activity coefficient model used to describe phase equilibria. This model belongs to a lattice model derived from a first-order approximation of interacting molecule surfaces in statistical thermodynamics. The model is, however, not fully thermodynamically consistent due to its two-liquid mixture approach. In this approach, the local concentration around one central molecule is assumed to be independent of the local composition around another type of molecule. The UNIQUAC model also serves as the basis for developing the group contribution method UNIFAC, where molecules are subdivided into functional groups. In fact, UNIQUAC is equal to UNIFAC for mixtures of molecules which are not subdivided, e.g. the binary systems water-methanol, methanol-acrylonitrile and formaldehyde-DMF.

Group	Component	Formula	CAS	Final yield [kg/kg biomass]
Proximate analysis				
	Carbonmonoxide	CO	630-08-0	0,05681
	Hydrogen	$H2$	1333-74-0	0,00813
	Methane	CH_4	74-82-8	0,00048
	Carbondioxide	CO_2	124-38-9	0,04693
	Ethane	C_2H_6	74-84-0	0,00196
	Propane	C_3H_8	74-98-6	0,00210
	Ammonia	NH_3	7664-41-7	0,00172
	Hydrogensulfide	$H2S$	7783-06-4	0,00075
Liquid / Oil				
	Phenol	C_6H_6O	108-95-2	0,04201
	Formic Acid	CH_2O_2	64-18-6	0,1001
	Formaldehyde	CH_2O	50-00-0	0,14865
	Glucose	$C_6H_{12}O_6$	50-99-7	0,05841
	Fluoranthene	$C_{16}H_{10}$	206-44-0	0,08807
	Dihydrogenoxide	H_2O	7732-18-5	0,17202
	Pyrolitic Lignin	NC	$CH_{1.1}O_{0.3}$	0,14285
Solid				
	Char	NC	$CH_{0.48}O_{0.23}$	0,12185
	Ash	NC	Ash	0,00716
Sum				1

Table 1.5: Characteristics of Biomass (pine sawdust)

The non-conventional components' properties need to be defined through values for HCOALGEN and DCOALLIGT.

In the Simulation section, Main Flowsheet, select a yield reactor and connect IN and Out streams. In the Setup sheet, set the Stream class to 'MIXNC'. This will enable the calculation of non-conventional components (go to Simulation-> set up-> specification-> Global setting stream class).

The next step is to define Biomass feed at 25 °C, 1 bar and 1 kg/s. Use Component Attribute is given in table 1.6a. The biomass stream enters the yield reactor, which represents the pyrolysis unit. The reaction works at the following conditions: 1[bar] and 500[°C]. The reaction yields are shown in table 1.6a. In the reactor block, the non-conventional product components need to be defined by their analyses according to tables 1.6b, 1.6c and 1.6d. The product compositions should be included in the "Comp. Attr." tab of the reactor unit.

The outlet stream from the reactor flows to the separator. The solid particles The SSPLIT assumes perfect separation of solid particles from the mainstream. Then the mixture of gaseous and liquid products enters the heat exchanger, which works at 30[°C] and 1[bar]. As a result, condensation occurs. The following step separates vapour from the liquid phase in a flash. The flash is assumed to be adiabatic and isobaric. The liquid stream is the main product and represents the bio-oil.

Group	Components	w-%
Moisture content	H_2O	10
Proximate analysis		
	Volatile matter (VM)	82.73
	Fixed carbon (FC)	16.47
	Ash	0.8
Ultimate analysis		
	C	50.64
	H	6.18
	O	42.22
	N	0.16
	S	0.08
	Ash	0.80
Sulfur analysis		
	Pyritic	0.0
	Sulfate	0.0
	Organic	0.08

(a) Biomass fuel analysis

Group	Components	w-%
Moisture content	H_2O	0
Proximate analysis		
	Volatile matter (VM)	80.00
	Fixed carbon (FC)	20.00
	Ash	0.0
Ultimate analysis		
	C	66.80
	H	6.18
	O	27.02
	N	0.0
	S	0.0
	Ash	0.0
Sulfur analysis		
	Pyritic	0.0
	Sulfate	0.0
	Organic	0.0

(b) The composition of lignin

Group	Components	w-%
Moisture content	H_2O	0
Proximate analysis		
	Volatile matter (VM)	80.00
	Fixed carbon (FC)	20.00
	Ash	0.0
Ultimate analysis		
	C	74.32
	H	2.99
	O	22.69
	N	0.0
	S	0.0
	Ash	0.0
Sulfur analysis		
	Pyritic	0.0
	Sulfate	0.0
	Organic	0.0

(c) The composition of char

Group	Components	w-%
Moisture content	H_2O	0
Proximate analysis		
	Volatile matter (VM)	0.00
	Fixed carbon (FC)	0.00
	Ash	100.0
Ultimate analysis		
	C	0.0
	H	0.0
	O	0.0
	N	0.0
	S	0.0
	Ash	100.0
Sulfur analysis		
	Pyritic	0.0
	Sulfate	0.0
	Organic	0.0

(d) The composition of char

Table 1.6: The composition of pyrolysis products

	Units	BIOMASS	BIOOIL	CHAR+ASH	COOLOUT	GAS	GAS+LIQ	R-OUT	S1
Description									
From			FLASH	SEPARATO	EA-1	FLASH	SEPARATO	DC-1RYIE	B1
To		DC-1RYIE	B1		FLASH		EA-1	SEPARATO	
Stream Class		MIXNC	MIXNC	MIXNC	MIXNC	MIXNC	MIXNC	MIXNC	MIXNC
Maximum Relative Error									
Cost Flow	$/hr								
− Total Stream									
Temperature	C	25	30	500	30	30	500	500	30
Pressure	bar	1	1	1	1	1	1	1	1
Mass Vapor Fraction		0	0	0	0.293757	1	0.835974	0.72805	0
Mass Liquid Fraction		0	0.767749	0	0.542217	0	0	0	0.767749
Mass Solid Fraction		1	0.232251	1	0.164026	0	0.164026	0.27195	0.232251
Mass Enthalpy	kcal/kg	-1553.33	-1725.08	-268.029	-1556.12	-1149.93	-1184.67	-1066.33	-1725.08
Mass Density	kg/cum	1266.25	1079.87	1518.11	2.85618	0.840595	0.536065	0.615498	1079.87
Enthalpy Flow	Gcal/hr	-5.59199	-3.81974	-0.124569	-4.87882	-1.05909	-3.71421	-3.83878	-3.81974
+ Mass Flows	**kg/hr**	**3600**	**2214.24**	**464.76**	**3135.24**	**920.999**	**3135.24**	**3600**	**2214.24**
+ Mass Fractions									
Volume Flow	cum/hr	2.84304	2.05047	0.306144	1097.7	1095.65	5848.62	5848.92	2.05047
− MIXED Substream									
Phase			Liquid Phase			Vapor Phase	Vapor Phase	Vapor Phase	Liquid Phase
Temperature	C		30		30	30	500	500	30
Pressure	bar	1	1	1	1	1	1	1	1
Molar Vapor Fraction			0		0.477811	1	1	1	0
Molar Liquid Fraction			1		0.522189	0	0	0	1
Molar Solid Fraction			0		0	0	0	0	0
Mass Vapor Fraction			0		0.351395	1	1	1	0
Mass Liquid Fraction			1		0.648605	0	0	0	1
Mass Solid Fraction			0		0	0	0	0	0
Molar Enthalpy	kcal/mol		-71.5735		-49.0161	-24.3637	-37.744	-37.744	-71.5735
Mass Enthalpy	kcal/kg		-2000.17		-1701.4	-1149.93	-1310.13	-1310.13	-2000.17
Molar Entropy	cal/mol-K		-45.2759		-21.7435	3.97449	4.6746	4.6746	-45.2759
Mass Entropy	cal/gm-K		-1.26527		-0.754741	0.18759	0.16226	0.16226	-1.26527
Molar Density	kmol/cum		28.9365		0.0829104	0.0396748	0.0155564	0.0155564	28.9365
Mass Density	kg/cum		1035.45		2.38858	0.840595	0.448168	0.448168	1035.45
Enthalpy Flow	Gcal/hr		-3.40026		-4.45934	-1.05909	-3.43383	-3.43383	-3.40026
Average MW			35.7836		28.8092	21.1871	28.8092	28.8092	35.7836
+ Mole Flows	**kmol/hr**	**0**	**47.5072**	**0**	**90.9771**	**43.4698**	**90.9771**	**90.9771**	**47.5072**
+ Mole Fractions									
− Mass Flows	**kg/hr**		**1699.98**		**2620.98**	**920.999**	**2620.98**	**2620.98**	**1699.98**
CO	kg/hr		0.210696		204.516	204.305	204.516	204.516	0.210696
H2	kg/hr		0.00334524		29.268	29.2647	29.268	29.268	0.00334524
CH4	kg/hr		0.00423811		1.728	1.72376	1.728	1.728	0.00423811
CO2	kg/hr		2.08479		168.948	166.863	168.948	168.948	2.08479
C2H6	kg/hr		0.119714		7.056	6.93629	7.056	7.056	0.119714
C3H8	kg/hr		0.493963		7.56	7.06604	7.56	7.56	0.493963
NH3	kg/hr		2.06668		6.192	4.12532	6.192	6.192	2.06668
H2S	kg/hr		0.105075		2.7	2.59493	2.7	2.7	0.105075
C6H6O	kg/hr		150.956		151.236	0.279673	151.236	151.236	150.956
CH2O2	kg/hr		351.921		360.036	8.1153	360.036	360.036	351.921
CH2O	kg/hr		70.7053		535.14	464.435	535.14	535.14	70.7053
C6H12O6	kg/hr		210.276		210.276	5.56162e-11	210.276	210.276	210.276
H2O	kg/hr		593.984		619.272	25.2883	619.272	619.272	593.984
C16H10	kg/hr		317.05		317.052	0.00177661	317.052	317.052	317.05
O2	kg/hr		0		0	0	0	0	0
N2	kg/hr		0		0	0	0	0	0
SO2	kg/hr		0		0	0	0	0	0
NO2	kg/hr		0		0	0	0	0	0
C	kg/hr		0		0	0	0	0	0
+ Mass Fractions									
Volume Flow	cum/hr		1.64177		1097.29	1095.65	5848.21	5848.21	1.64177
+ Vapor Phase									
+ Liquid Phase									
− NC Substream									
Temperature	C	25	30	500	30		500	500	30
Pressure	bar	1	1	1	1	1	1	1	1
Mass Enthalpy	kcal/kg	-1553.33	-815.699	-268.029	-815.699		-545.207	-413.625	-815.699
Mass Density	kg/cum	1266.25	1258.31	1518.11	1258.31		1258.31	1369.57	1258.31
Enthalpy Flow	Gcal/hr	-5.59199	-0.419481	-0.124569	-0.419481		-0.280378	-0.404947	-0.419481
− Mass Flows	**kg/hr**	**3600**	**514.26**	**464.76**	**514.26**	**0**	**514.26**	**979.02**	**514.26**
BIOMASS	kg/hr	3600	0	0	0	0	0	0	0
ASH	kg/hr	0	0	26.1	0	0	0	26.1	0
CHAR	kg/hr	0	0	438.66	0	0	0	438.66	0
LIGNIN	kg/hr	0	514.26	0	514.26	0	514.26	514.26	514.26

Figure 1.5: Fast pyrolysis results

Chapter 2

Process analysis

Following the work of [1], let's analyse the esterification of lactic acid with methanol given by the following chemical reaction

$$\underbrace{CH_3CHOHCOOH}_{Lactic\ Acid} + \underbrace{CH_3OH}_{Methanol} \rightarrow \underbrace{CH_3CHOHCOOCH_3}_{Methyl\ Lactate} + \underbrace{H_2O}_{Water} \tag{2.1}$$
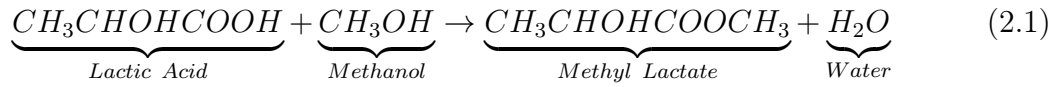
The simplified process flow diagram, is presented on Figure 2.1.
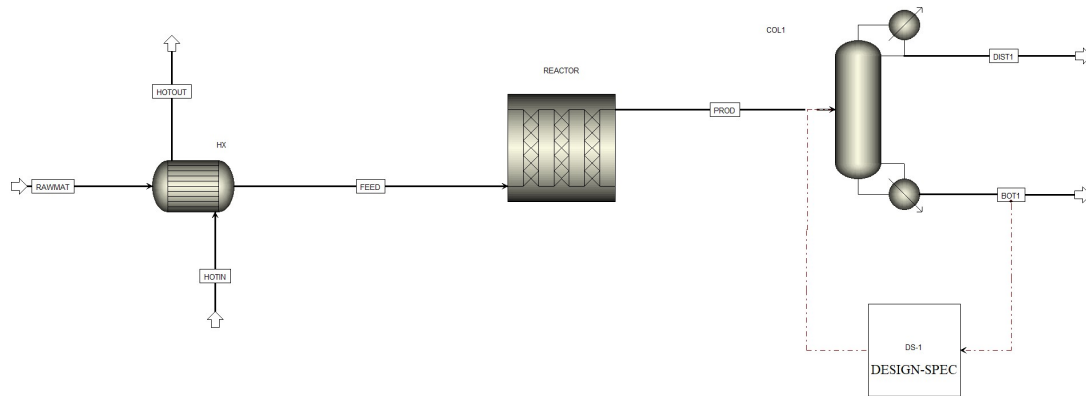
Figure 2.1: Process flow diagram

The kinetic model is used to represent the reaction rate, but the effect of the reverse reaction is neglected. Thus, the reaction rate is expressed as follows:

$$r = k_1 \exp\left(\frac{-E_a}{RT}\right) a_{LACTIC}^2 a_{MeOH} \tag{2.2}$$

where k_1 is equal to 6.024×10^8 $[mol \cdot min^{-1}]$, E_A is equal to 56.45 $[kJ \cdot mol^{-1}]$, and a_i is the activity of the component i.

2.1   Initial simulation

The thermodynamics is calculated based on the UNIFAC method. In statistical thermodynamics, the UNIFAC method (UNIQUAC Functional-group Activity Coefficients) is a semi-empirical system for predicting non-electrolyte activity in non-ideal

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mixtures. UNIFAC uses the functional groups present on the molecules that make up the liquid mixture to calculate activity coefficients. The activity of each of the solutions can be calculated by using interactions for each of the functional groups present on the molecules and some binary interaction coefficients. The UNIFAC correlation attempts to break down the problem of predicting interactions between molecules by describing molecular interactions based on the functional groups attached to the molecule. This is done in order to reduce the sheer number of binary interactions that would be needed to be measured to predict the state of the system.

Let's initiate the simulation by setting up the reactor block first. In this case, 100 $[kmol/h]$ of lactic acid is allowed to enter a tubular reactor. Methanol is also fed to the reactor, with a methanol/lactic acid mole ratio of $3:1$. The reactor operates at 340 $[K]$ and 1 $[bar]$. Esterification of lactic acid occurs inside the vessel; thus, the stream leaving the equipment contains methyl lactate, water, and unreacted methanol and lactic acid. The reaction occurs in a Plug Flow Reactor (PFR). The first parameter to be decided is the characteristic of the reactor, which in this case is set to *reactor with specified temperature*, which means that the feed temperature determines the reactor's temperature. To set the initial simulation the reactor length is assumed to be 5 $[m]$, and the diameter to be 0.1 $[m]$.

Because the kinetic model is provided as a power law, the reaction type is selected as *POWERLAW*. The coefficients of the reactants (lactic acid and methanol) are set as -1, and the coefficients of the products (methyl lactate and water) are set as 1. The exponent is defined as 2 for lactic acid and 1 for methanol because it is the power for each component activity in the kinetic expression. The products are not involved in the kinetic model for the straight reaction. Thus, the field is left blank, which implies an exponent of 0. The values for the pre-exponential factor k_1 and the activation energy E_a are known. The reference temperature T_0 is not specified; the exponent n is set as 0 to allow temperature dependence to be modelled using the Arrhenius equation. Finally, the basis for concentration is selected as Mole gamma to allow the kinetic calculations to be based on the activities of the component.

The simulation results presented in Table 2.1.

		Feed	Product
Mole Flows	kmol/hr	400	400
LACTI-01	kmol/hr	100	96.73
METHA-01	kmol/hr	300	296.73
METHY-01	kmol/hr	0	3.268
WATER	kmol/hr	0	3.268
Mole Fractions			
LACTI-01		0.25	0.24
METHA-01		0.75	0.74
METHY-01		0	0.0082
WATER		0	0.0082

Table 2.1: Initial simulation results
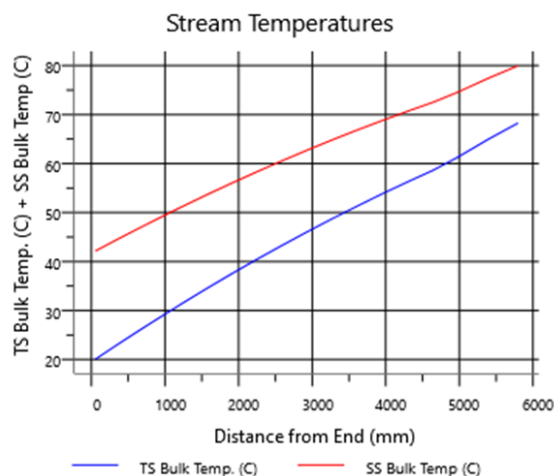
This reaction is characterized by low conversion to methyl lactate ($\approx 3.3\ mol\%$). The reactor design is considered inefficient enough to convert to methyl lactate.
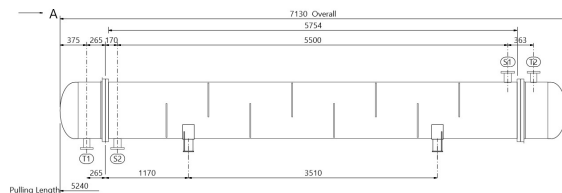
2.2 Heat Exchangers

Let's assume that the reactants' temperature is not 340[K] as specified before, but 293 [K]. Therefore, a heat exchanger is needed to raise the temperature of the inlet stream. As the temperature difference is relatively low, we assume that the thermal fluid is hot water (temperature 353 [K] and flowrate equal 1000 [kmol/h]). The *HeatX* module will be used in this simulation. First, the shortcut calculations are performed to set *Cold stream outlet temperature* to be 340 [K]. Then, the *Shell & Tube* type of heat exchanger is selected to perform more detailed calculations. Remember, the more precise calculations might be characterised by lower efficiency than the shortcut calculations, for example, by considering a pressure drop. We use interactive sizing is used to find the heat exchanger geometry. Luckily, there is no error; nevertheless, some warnings are present. For simplicity, we will modify the simulation to decrease the pressure drop to a minimum (0.07 [bar]), as we

(a) Stream temperatures along the heat exchanger

(b) External dimension of the heat exchanger

Figure 2.2: Results of heat exchanger design

do not simulate pumps in this work. However, checking if the pressure drop doesn't force a phase change is always recommended.

In non-conventional cases, each heat exchanger section might be specified by assigning a specific TEMA-type equipment.

The suggested design is a classic Shell&Tube heat exchanger with one pass. Figure 2.2 shows the final result of the heat exchanger design.
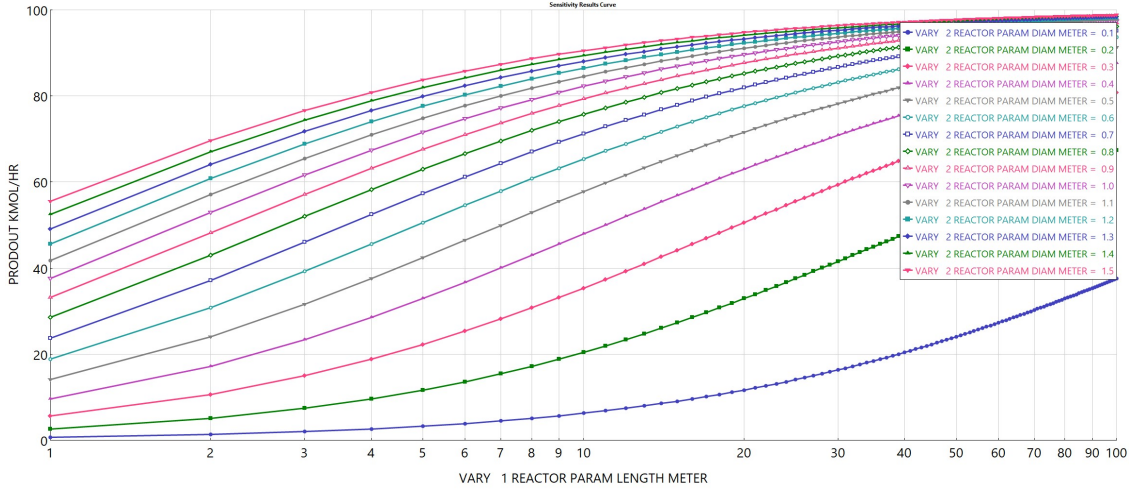
2.3 Sensitivity Analysis

The *sensitivity analysis* allows evaluating a parameter's influence on model output. In this case, the reactor's diameter and length are selected as degrees of freedom and can be manipulated. The system output is the amount of the methyl lactate at the reactor outlet.

In *Vary* section, two variables are created: one corresponds to the length of the reactor, while the second one is the diameter of the reactor. Both variables are *Block-Var* Type. Let the length change from 1 [m] to 100 [m] every 1[m], and the diameter change from $0.1 - 1.5$ [m] every 0.1 [m]. In *Define* section, model output is defined. The model output is affected by a change from *Vary* section. The output variable, in this case, is the mole flowrate of methyl lactate in the outlet stream.

The mole flowrate can be found in the *Streams* category. The sensitivity analysis results are in Figure 2.3.
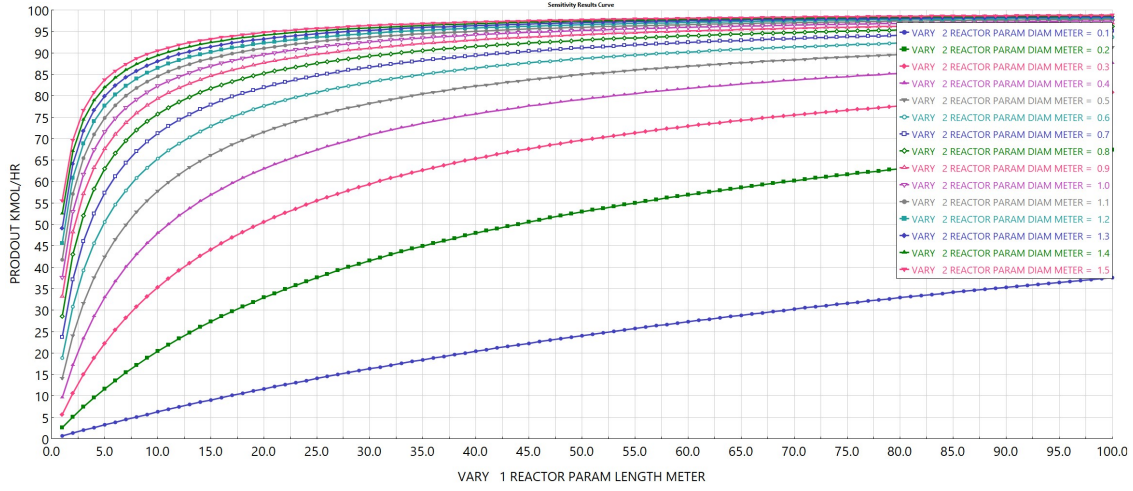
(a) Sensitivity analysis - linear scale

(b) Sensitivity analysis - log scale

Figure 2.3: Sensitivity analysis results

As shown in Figure 2.3, the initial value of reactors length and diameter are insufficient to obtain high conversion.

The next step is defining a local variable describing lactic acid's conversion. Three variables need to be defined in the *Define* section. Two variables describe the molar flowrate of lactic acid at the inlet and the outlet stream, and the third one describes the conversion rate. The molar flowrates can be found in the *Streams* category. The conversion is defined as *Local-Param*, but the conversion formula should be written in the *Fortran* section.

Be careful to use the symbols in the exact form as they are defined in the *Define* page. The conversion can be calculated from the following equation:

$$CON = \frac{(FEED - PRODUCT)}{FEED} \cdot 100\% \tag{2.3}$$

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The results of the sensitivity analysis conducted with respect to the conversion are presented in Figure 2.4.
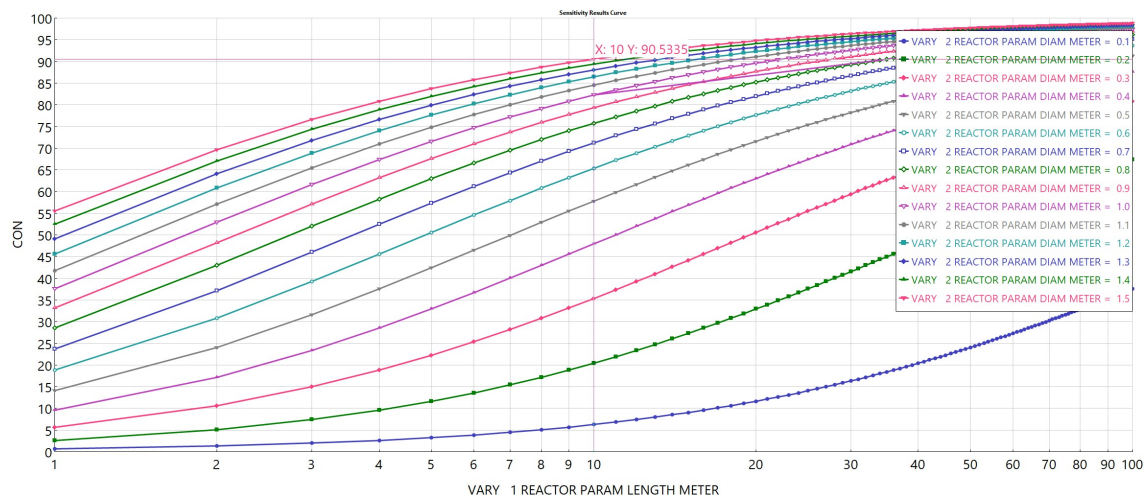

Figure 2.4: Sensitivity analysis with respect to conversion

Based on the sensitivity analysis, we select the first value, which gives us the conversion of 90%, so the length of 10 [m] and the diameter of 1.5 [m]. Any reasoning can be applied to select the reactor size. One can perform a similar analysis with respect to any indicator and use it to draw a conclusion.

2.4 Design-spec

Let's investigate how to separate compounds of the stream leaving the reactor. By analysing singular points from the Distillation Synthesis Analysis (Table 2.2), it can be noticed that there is one azeotrope.

	Temp (C)	Classification	Type	No. Comp.	LACTI-01	METHA-01	METHY-01	WATER
1	216.627	Stable node	Homogeneous	1	1.000	0.000	0.000	0.000
2	64.535	Unstable node	Homogeneous	1	0.000	1.000	0.000	0.000
3	144.813	Saddle	Homogeneous	1	0.000	0.000	1.000	0.000
4	100.018	Saddle	Homogeneous	1	0.000	0.000	0.000	1.000
5	99.855	Saddle	Homogeneous	2	0.000	0.000	0.027	0.973

Table 2.2: Singular points from the Distillation Synthesis Analysis

The same conclusion can be drawn form of the ternary plot (Figure 2.5).
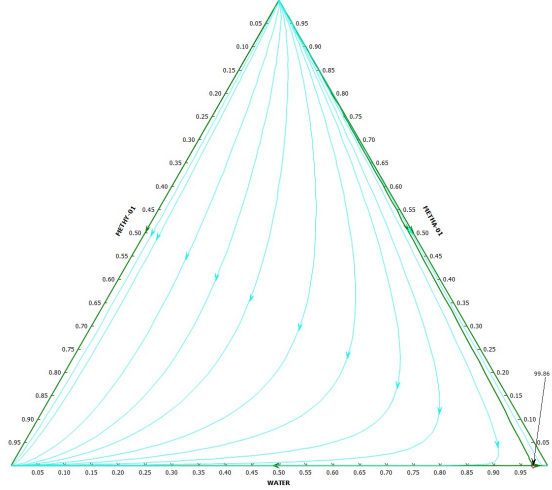
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Figure 2.5: Ternary plot

In this simulation work, we are going to remove non-azeotropic components first. We start with *METHA-01*, one of the reactants with the lowest boiling point. The distillation column is modelled with *RadFrac* module. We assume the number of stages to be 30 and the feed stage to be 15. The distillation column is characterized by the Distillate rate equal to the mole flowrate of the *METHA-01*, and the molar reflux ratio equal to 1. The *Design-spec* is used to increase the bottom stream's purity. It is assumed that the number of stages, the feed stage and the distillate rate are fixed, but the reflux ratio can be manipulated. The *Design-spec* can be found in the *Flowsheeting Option* folder. First, the model output needs to be defined. In this case, the model output is the mole fraction of acetic acid in the bottom stream. In the *Spec* section, the target value of the model output is specified. We assume that the bottom stream should have the molar fraction of the acetic acid equal to $1e - 4$, with tolerance $1e - 5$. The next step is to define what parameter can be used to tune the model output. In this case, we used the molar reflux ratio, which can vary from 0.5 to 2. The adjusted value of the reflux ratio is 1.5524972, and simulation results can be found in Table 2.3.

		Product	Distillate	Bottom
Mole Flows	kmol/hr	400	190.51	209.5
LACTI-01	kmol/hr	9.467	9.467	4.82E-50
METHA-01	kmol/hr	209.467	0.019	209.45
METHY-01	kmol/hr	90.53	90.53	2.61E-16
WATER	kmol/hr	90.53	90.48	0.053
Mole Fractions				
LACTI-01		0.023	0.050	2.30E-52
METHA-01		0.523	0.0001	0.9997
METHY-01		0.226	0.476	1.2450E-18
WATER		0.226	0.475	0.000251

Table 2.3: Stream results of the distillation column

2.5 Column Internals

The next step is to analyse the distillation column from the hydraulic point of view. The fact that the simulation of the distillation column has converged and satisfies the mass balance doesn't mean that the hydraulics are well designed. This requires special attention and separate analysis. The analysis tools for a column hydraulic can be found in the *Column Internals* folder. One can use the *Auto Section* option to create different sections along the column. In this case, the software suggests two sections of different diameters (both with sieve trays). One section is above, and the second is below the feed stage. The results of the auto-section tool are given in Table 2.4.

Name	Start Stage	End Stage	Mode	Internal Type	Tray/Packing Type	Number of Passes	Tray Spacing/Section Packed Height	Dimension	Diameter	Dimension
CS-1	2	14	Interactive sizing	Trayed	SIEVE	1	0.6096	meter	1.608	meter
CS-2	15	29	Interactive sizing	Trayed	SIEVE	1	0.6096	meter	1.596	meter

Table 2.4: Column design given by automatic tool

The graphical representation of the this column is presented on Figure 2.6
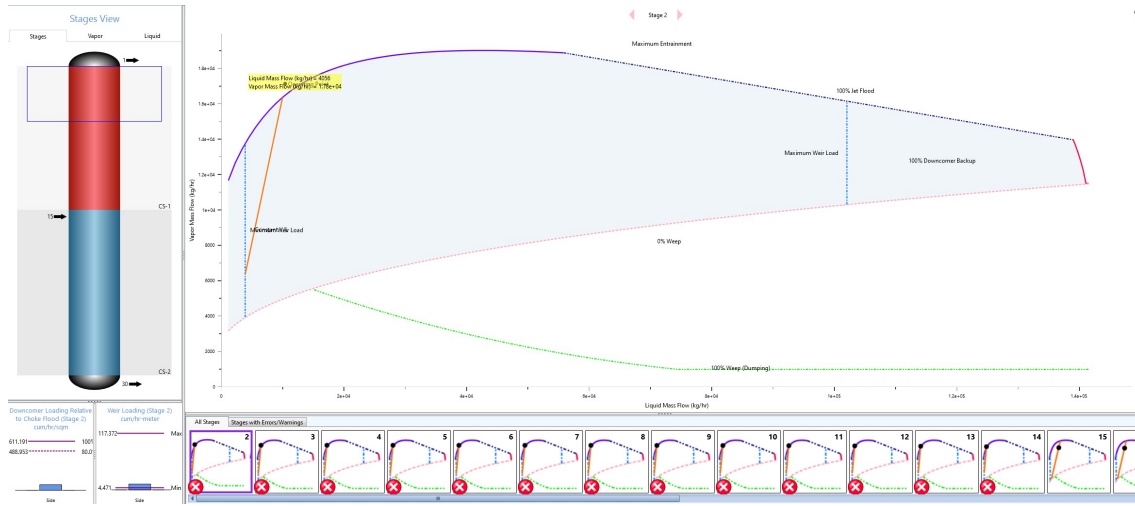

Figure 2.6: Column internals

The software returns the following error "Entrainments on Stages 2 - 14 are above the specified maximum percent liquid entrainment of 10. We recommend increasing tray spacing." First, both sections have almost the same diameter (1.6 [m]), so the whole column can be represented by one section. The error given by the software can be solved by increasing the spacing from the default value of 0.6096 [m] to 0.75 [m]. Figure 2.7 presents the corrected column hydraulic.

Figure 2.7: Column internals

Chapter 3

Economic Analysis

3.1 Acetic anhydride production

We use the production of acetic anhydride from acetone to demonstrate how to evaluate the economic attributes of a chemical process. We are going to follow the book of [2]. The process flowsheet for acetic anhydride production is made of PFR with a recycle for the unreacted acetone, followed by two downstream separation units: rectifying and distillation column and finally, the conversion of ketene and acetic acid into acetic anhydride using CSTR. The flowsheet is presented on Figure 3.1
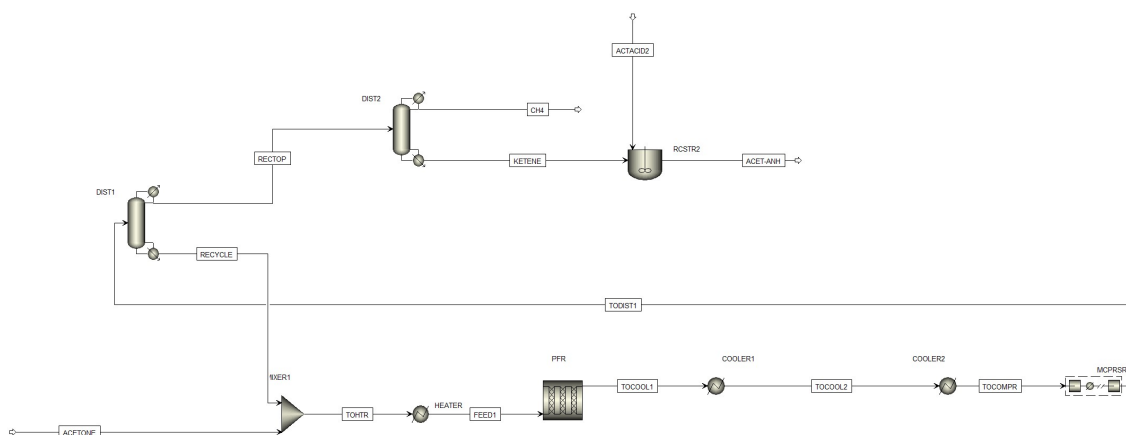
Figure 3.1: The process flowsheet for acetic anhydride production with recycling of the unreacted acetone

The methods recommended by Aspen for Carboxylic Acids are activity coefficient methods with Nothangel or Hayden-O'Connel model with vapour phase association with NRTL-HOC or WILSON-NTH. In this simulation, Wilson-NTH is chosen.

All the missing binary interaction coefficients can be estimated by the UNIFAC method, which uses information about the structure of particular components to predict their behaviour.

The reactor design in Aspen Plus depends on the reactor type the user chooses. In this exercise, the PFR and CSTR reactors are used. The first reactor is PFR. Firstly, one needs to decide on the reactor type. The adiabatic reactor is used in

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this case. Then the reactor dimensions should be provided. The third step is to define the kinetics of the reaction need to be defined. The powerlow model is used. Kinetic data can be found in [3].

The outlet stream from the reactor contains a high amount of unreacted acetone, which should be separated and recirculated. This can be done with an absorption column or distillation column.

Although, the vapour feed to the column should be compressed before the separation. The 4-stage compressor can be used for that purpose. Then the stream is fed into the column. This is an example of a rare process which belongs to the cryogenic group due to the significantly lower temperature in the condenser. The acetone is a bottom product and is recycled. The methane is separated from ketene in a distillation column in the second column. The ketene is a bottom product of the distillation and is used as a feed for the CSTR reactor. The ketene is mixed with acetic acid in the reactor. First, the information about working conditions (T and P) and the reactor's technical details (Volume) must be introduced to Aspen Plus. Then the reaction is described. The powerlaw model is used again, but the reaction type is "equilibrium", meaning that the Gibbs energy minimization algorithm is used.

The input file can be found at the end of this chapter. The results of the simulation are presented in table 3.1:

	Units	ACET-ANH	ACETONE	ACTACID2	CH4	FEED1	KETENE	RECTOP	RECYCLE	TOCOMPR	TOCOOL1	TOCOOL2	TODIST1	TOHTR
Temperature	C	7.50E+01	2.50E+01	2.50E+01	-9.79E+01	7.62E+02	5.59E+01	-6.05E+01	2.03E+02	9.00E+01	6.28E+02	1.40E+02	1.95E+02	7.01E+01
Pressure	bar	1.50E+01	1.60E+00	1.50E+01	2.80E+01	1.60E+00	2.80E+01	2.90E+01	2.90E+01	1.60E+00	1.60E+00	1.60E+00	2.90E+01	1.60E+00
Mole Flows	kmol/hr	1.72E+01	1.72E+01	1.71E+01	1.72E+01	7.37E+01	1.72E+01	3.44E+01	5.65E+01	9.09E+01	9.09E+01	9.09E+01	9.09E+01	7.37E+01
CH_3COCH_3	kmol/hr	1.22E-02	1.72E+01	0.00E+00	4.92E-32	7.37E+01	1.22E-02	1.22E-02	5.65E+01	5.65E+01	5.65E+01	5.65E+01	5.65E+01	7.37E+01
C_2H_2O	kmol/hr	7.94E-02	0.00E+00	0.00E+00	2.82E-14	1.22E-02	1.72E+01	1.72E+01	1.22E-02	1.72E+01	1.72E+01	1.72E+01	1.72E+01	1.22E-02
CH_4	kmol/hr	1.72E-02	0.00E+00	0.00E+00	1.72E+01	1.72E-12	1.72E-02	1.72E+01	1.72E-12	1.72E+01	1.72E+01	1.72E+01	1.72E+01	1.72E-12
CH_3COOH	kmol/hr	1.16E-05	0.00E+00	1.71E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ACET-ANH	kmol/hr	1.71E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
H_2O	kmol/hr	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mole Fractions														
CH_3COCH_3		7.08E-04	1.00E+00	0.00E+00	2.86E-33	1.00E+00	7.08E-04	3.54E-04	1.00E+00	6.21E-01	6.21E-01	6.21E-01	6.21E-01	1.00E+00
C_2H_2O		4.61E-03	0.00E+00	0.00E+00	1.64E-15	1.66E-04	9.98E-01	5.00E-01	2.16E-04	1.89E-01	1.89E-01	1.89E-01	1.89E-01	1.66E-04
CH_4		9.98E-04	0.00E+00	0.00E+00	1.00E+00	2.33E-14	9.98E-04	5.00E-01	3.04E-14	1.89E-01	1.89E-01	1.89E-01	1.89E-01	2.33E-14
CH_3COOH		6.76E-07	0.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ACET-ANH		9.94E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
H_2O		0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table 3.1: Simulation result of the acetic anhydride production

3.2   Economic analysis steps

If we have the process simulation ready and stable, we can move to the economic analysis of the process. The economic analysis requires defining feed and product stream prices, defining utilities in terms of pricing, and associating them with equipment such as a pump, compressor, condenser, reboiler, and heater. The economic analysis consists of several steps.

Step 1: Investment options

In "Navigation" panel, let us go to "Setup" | "Costing Options" | "Costing options" tab form to specify "operating life of plant", "length of plant startup" and "start of basic engineering".

Step 2: Feed, product and utility prices

In the "Setup" | "Stream Price" | "Input" form, the price per unit of the feed or product stream can be specified. In the "Utilities" folder, each utility used in the simulation is characterized. Each pre-defined utility has its own "purchase price" or "energy price". The price of a utility can be modified by entering detailed information about that utility. The prices used in this exercise are shown in table 3.2, and the utility prices have default values suggested by the software.

Stream ID	Source	Destination	Basis	Price	Unit
ACET-ANH	RCSTR2		Mass	1000	\$/tonne
ACTACID2		RCSTR2	Mass	600	\$/tonne
ACETONE		MIXER1	Mass	1200	\$/tonne
CH4	DIST2		Mass	6150	\$/tonne

Table 3.2: Feed and product prices

Step 3: Activation of the economical module

There are two routs to perform economic analysis with Aspen environment. First one is to use the economic module, which is incorporated in the Aspen Plus software. The second one is to use stand-alone module called "Aspen Economic Analyzer" (APEA). We are going to focus on the second method as it is more comprehensive and give more flexibility.

Nevertheless which method is used, the general steps are the same: "Mapping", "Sizing" (Step 4) and "Evaluation" (Step 6). Details on each step will be covered in the following text.

The first step is to send the process simulation to the APEA. It can be done with "Send to APEA" button in the "Economics". Next, a new project needs to be created. Then the simulation data can be loaded, but special attention needs to be paid to check if correct fluid are associated to each utility. In this case, "AIR" utility should associated with air fluid, "FH100" utility with high-temperature hot oil, and "REFRIG4" with refrigerant ethane.

The details of the economic variables can be found in the "Project Basis View". The list of equipment is located in the "Process View" section. In case of need, more pieces of equipment can be added in this section directly (so it is not needed to go back to the process simulation).

Step 4: Mapping and sizing

The "Map option" can be activated with the "Map simulator Items" button at the top of the page. The "Size equipment" should be marked, while "Custom sizing" can be left unmarked. The "Customize sizing" option interferes with equipment sizing details and allows to use of custom sizing models. In the "Map Preview" window, all the flowsheet objects are mapped with APEA built-in objects. For example, we are going to use the following mapping:

(a) COOLER1 is "Floating headshell and tube exchanger" because of a significant temperature difference between the hot and cold stream.

(b) COOLER2 is "Air cooler" to reflect that "AIR" utility is used.

(c) DST1(RADFRAC) and DST2(RADFRAC); The distillation columns consist of the sets of equipment, and each should be specified.

- Tower type is "Multiple diameters, trayed or packed tower".
- Condenser type is "Bare pipe immersion coil".
- Condenser drum is a "Horizontal drum".
- Reflux pump type is "Centrifugal single or multi-stage pump".

(d) Heater type is "Box type process furnace".

(e) Mixer can be represented as "Agitated tank – enclosed".

(f) The compressor type is "Centrifugal compressor - horizontal".

(g) PFR is "Packed tower".

(h) CSTR is "Agitated tank – enclosed, jacketed".

The mapping and sizing are performed automatically.

Step 5: Debugging

The next step would be to evaluate the project by clicking the "Evaluate Project" button. If things go smoothly, you will reach the final executive summary for costs without hassles, and you can go to the Step 6. However, you may get a warning or error message during the evaluation step regarding sizing or missing input data for some pieces of equipment. To check for issues, you can look at the generated report to find that APEA reports errors due to improper entry, such as the type of construction material or a property value that is out of range. On the other hand, the warning message alarms the user that an error might be incurred in the user's selected mapped object specifications.

- HEATER

  ERROR> 'FU - 5' STRESS FOR MATERIAL A 214 IS ZERO AT A TEMPERATURE OF 791.85 SYSTEM MAY NOT CONTAIN STRESS VALUES FOR THE MATERIAL.

  This means that construction A214 (Carbon Steel) material is unsuitable for a high-temperature heater. However, the default Carbon steel A214 can be replaced with S347.

  Each piece of equipment can be modified in the "Project View" section. Right-click on an item and select modify to access the details of each piece of equipment. After changes, the inner "Evaluate" use a button to evaluate only a selected item.

- PFR

  *Component Item Description: PFR User Tag Number: PFR *Component Ref #: 2 WARN > 'TW - 2' PACKING TYPE ' ' AND/OR VOLUME INCORRECT.*

If we use "1.0 CRR Ceramic raschig ring" as the "Packing type".

- COOLER 1

  Component Item Description: COOLER1 User Tag Number: COOLER1 *Component Ref #: 17 WARN > 'HE - 17' DESIGN TEMPERATURE TOO HIGH FOR VACUUM OR EXTERNAL PRESSURE DESIGN

  COOLER1 material can be specified as "347S" and "SS347" for both tube and shell construction.

Step 6: Project evaluation

Clicking on "Capital Costs" o generate a full-fledge report s that includes all cost-based technical project details, including design, equipment, civil, structural, piping, mechanical, steel, instrumental, electrical, insulation, paint, labor, management, and the project metrics, such as Independent Project Analysis (IPA) metrics and Project Evaluation System (PES) summary and cost check.

The investment analysis of the project is summarized in table 3.3.

The summary of the overall cost obtained from the economic analysis can be found in table 3.4.

Remember that total operating cost includes:

- Total raw materials cost
- Total utilities cost
- Operating labor cost
- Maintenance cost
- Operating charges
- Plant overhead
- Subtotal operating cost
- General and admin cost

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.75
DT (Duration of EPC Phase and Startup)	Period	1.13462
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	1.35E+07
RAWT (Total Raw Material Cost)	Cost/period	1.45E+07
PRODT (Total Product Sales)	Cost/period	2.76E+07
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.36E+06
UTILT (Total Utilities Cost)	Cost/period	547531
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
PODE (Desired Payout Period (excluding EPC and Startup Phases))	Period	
POD (Desired Payout Period)	Period	
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.480769
OP (Total Operating Labor Cost)	Cost/period	1.24E+06
MT (Total Maintenance Cost)	Cost/period	115000

Table 3.3: Summery of the investment analysis

INVESTMENT:		
Currency Conversion Rate	1.00	USD/U.S. DOLLAR
Total Project Capital Cost	13'450'400.00	USD
Total Operating Cost	18'820'400.00	USD/Year
Total Raw Materials Cost	14'536'300.00	USD/Year
Total Utilities Cost	547'531.00	USD/Year
Total Product Sales	27'587'800.00	USD/Year
Desired Rate of Return	20.00	Percent/'Year
P.O. Period	5.83	Year

Table 3.4: Overall costs of the acetic anhydride production

3.3 Investment indicators

An economy of an arbitrary process can be analysed based on different indicators. The most popular indicator is the **Net Present Value (NPV)**, which applies to

a series of cash flows occurring at different times and accounts for the "time value of money". NPV is determined by calculating the costs (negative cash flows) and benefits (positive cash flows) for each period of an investment. After the cash flow for each period is calculated, the present value (PV) of each one is achieved by discounting its future value (see equation 3.1) at a periodic rate of return (the rate of return dictated by the market). NPV is the sum of all the discounted future cash flows, as given by equation 3.2.

$$PV = \frac{R_t}{(1+r)^t} \tag{3.1}$$

$$NPV = \sum_{i=0}^{N} \frac{R_t}{(1+i)^t} = \sum_{i=0}^{N} PV \tag{3.2}$$

where t is the time of the cash flow, r is the discount rate, i.e. the return that could be earned per unit of time on investment with similar risk, and R_t is the net cash flow, i.e. cash inflow – cash outflow, at time t and N is the number of time intervals.

Based on the project evaluation performed in Step 6, the PV and NPV are found. The PV and NPV curves are presented in Figure 3.2.
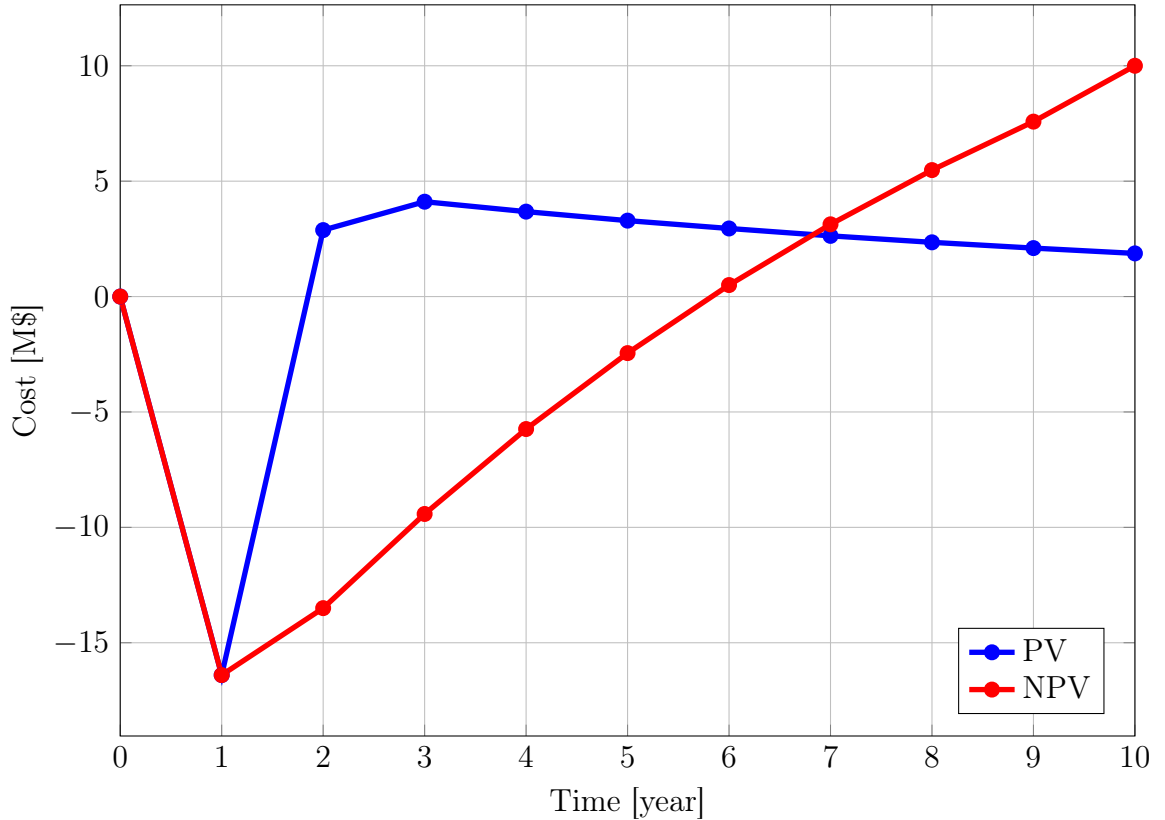

Figure 3.2: Cash flow

NPV is negative for the first six years and becomes positive afterwards, meaning the project appears profitable from year seven onward.

The second indicator is the **discounted payout period (DPP)**, which is described by equation 3.3

$$DPP = \text{Years with negative NPV} + \frac{|\text{NPV}|}{\text{PV}} = 5 + \frac{|-2.45E+06|}{2.95E+06} = 5.83 \text{ years} \qquad (3.3)$$

DPP represents the length of time required to recover the cost of an investment. The payout (or, payback) period of a given investment project is an important determinant of whether to undertake the project, as longer payback periods are typically not desirable for investment projects. Notice that the payout period indicator ignores any benefits that occur after the payback period and, therefore, does not measure profitability. In addition, it ignores the time value of money.

The third indicator is the **profitability index (PI)** that shows the present value of the benefits relative to the present value of the costs. The PI is defined as given by equation 3.4

$$PI = \frac{\text{Present Value of the Cumulative Cash Inflows (PVI)}}{\text{Present Value of the Cumulative Cash Outflows (PVO)}} \qquad (3.4)$$

If the profitability index is greater than one, then the project appears to be profitable. If this index is less than one, the project appears unprofitable. If this number equals one, the project incurs no losses or gains (break-even point). PI's time evolution is shown in Figure 3.3.
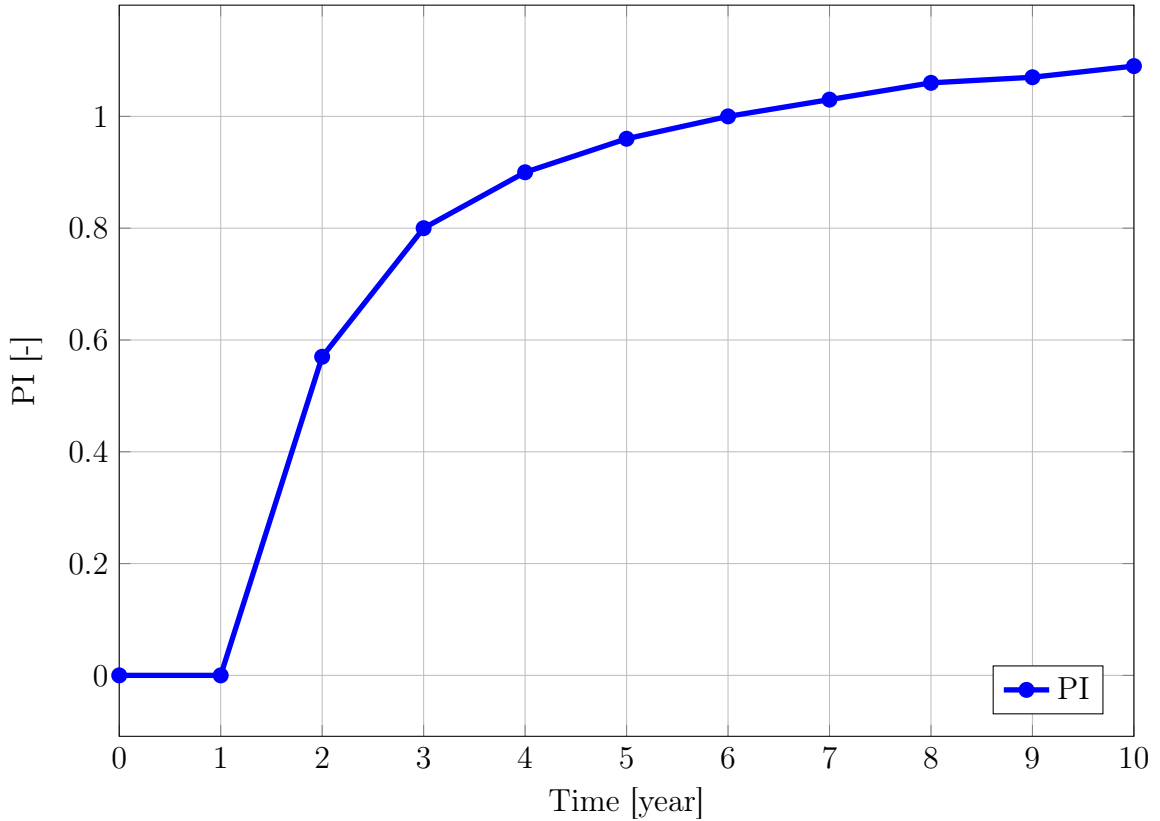

Figure 3.3: Profitability index

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The fourth indicator is the **internal rate of return (IRR)**. The internal rate of return (IRR) is the discount rate at which the net present value of an investment becomes zero. In more specific terms, the IRR of an investment is the discount rate at which the net present value of costs (negative cash flows) of the investment equals the net present value of the benefits (positive cash flows) of the investment. In this case, the $IRR = 34.27\%$. A project should only be accepted if its IRR is NOT less than the target internal rate of return. When comparing two or more mutually exclusive projects, the project with the highest value of IRR should be considered.

The fifth indicator is the **modified internal rate of return (MIRR)**. IRR assumes that positive cash flows are reinvested at the same rate of return as the investments (i.e., the project which generates them). This assumption is questionable as funds are reinvested at a rate that reflects the organization's cost of capital or returns on cash. Consequently, if we stick with the assumption of an equal rate for both negative and positive cash flow, IRR gives an optimistic (i.e., overestimated) rate of return for the cash flows. In addition, more than one IRR may be found for projects with alternating positive and negative cash flows, leading to confusion. Two interest rates are needed to use MIRR: The reinvestment rate for the positive cash flow (PV) and the finance rate for the negative cash flow (NV). The MIRR is given by equation 3.5.

$$MIRR(\%) = \left[\left[\frac{FV}{-PV} \right]^{\frac{1}{EPELP}} - 1 \right] \times 100\% \qquad (3.5)$$

where EPELP is the "End Period for Economic Life of Project" (i.e., EPELP=10 years, by default), PV is the sum of cash flows (brought to the beginning of the first period), and FV is the sum of positive cash flows (brought to the end of the last period).

The MIRR value was found to be 21.03%, which is less than IRR.

3.4   APEA without process simulation

It is not always possible to simulate a whole production process with Aspen Plus, particularly in bio-based processes. The APEA can be used to estimate an equipment price based on a limited amount of information from hand-made calculations. To use the APEA without the process simulation, select a piece of equipment from the *Process equipment* section. *Process equipment* section is usually located in the top-right corner in the *Components* tab (Figure 3.4). Then, an analysed equipment needs to be added in the *List* section by drag-and-drop. The selection of equipment from *Process equipment* section corresponds to the mapping procedure discussed before. The drag-and-drop will cause the opening of new windows called *New Component information*, where the name of the analyzed machine needs to be assigned. After acceptance of the equipment name, a new window with a technical sheet will open.
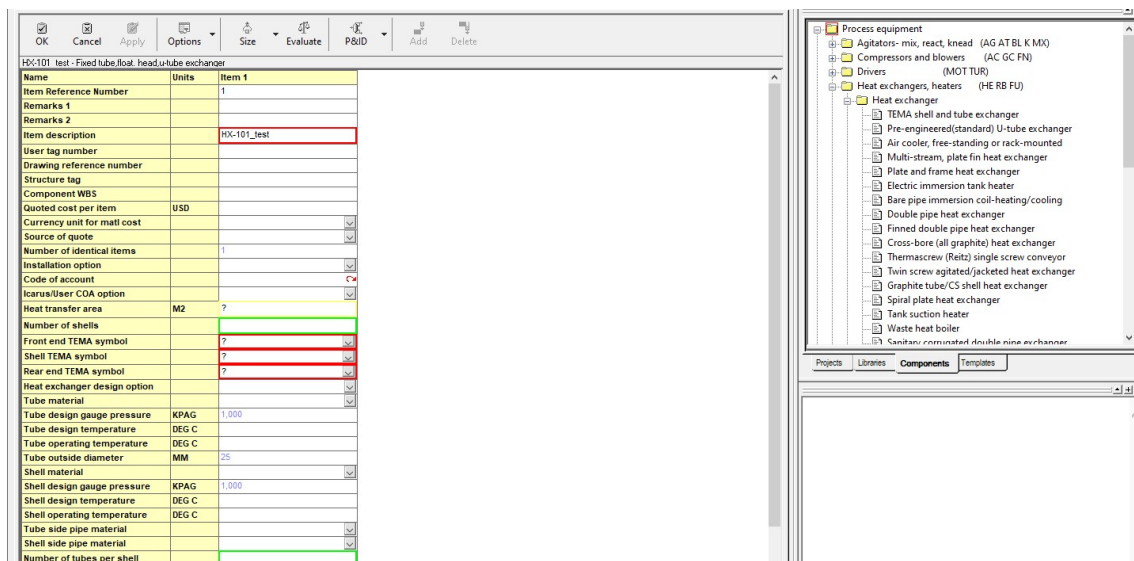
Figure 3.4: Equipment selection

The tab with a heat exchanger is presented on the right-hand side of Figure 3.4. Necessary pieces of information for the cost estimation are highlighted. In this case, a heat transfer area needs to be known a priori. In addition to the heat transfer area, TEMA symbols representing the front end, the shell, and the rear end need to be selected. The selection of TEMA symbols differs from case to case and should be justified.

When all the necessary pieces of information are included, the *Apply* button is used to save the changes. Let's assume that the heat transfer is $10m^2$ and the TEMA symbols are A, E, and L. The *Evaluate* button is used to prepare a report that summarizes all the costs related to the equipment, as presented in Table 3.5. If a percentage method is used in the student's report to estimate the plant cost, then the *equipment and setting* should be used.

	MATERIAL	MANPOWER	MANPOWER
	USD	USD	MANHOURS
EQUIPMENT&SETTING	14700	954	29
PIPING	19406	12387	366
CIVIL	1214	1724	63
STRUCTURAL STEEL	0	0	0
INSTRUMENTATION	12366	4251	124
ELECTRICAL	0	0	0
INSULATION	6622	5630	219
PAINT	405	1090	43
SUBTOTAL	54714	26036	844
INSTALLED DIRECT COST	80800		

Table 3.5: The cost estimation example

Additional modifications might be necessary as an equipment design changes from case to case. If an operating temperature or pressure differs from the stan-

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dard conditions, then the appropriate change in the *design temperature* and *design pressure* sections should be implemented. For instance, the change in operating pressure affects the wall thickness, which further influences the equipment. The materials used to build equipment should be selected depending on the reactants. If there are some corrosive substances, then *material* should be used to select the appropriate material.

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