Aspen Tutorials

Plant Design Group, Aalto University
Oliwer Sliczniuk

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Preface

The research in Plant Design focuses on process feasibility study, synthesis, design, operation, integration, simulation and optimization, as well as 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 that are applicable in all areas of chemical process industry. 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 the development of new processes, engineering of new plants and improvement of existing ones in the chemical, petrochemical, biofuel, pulp and paper, minerals, food and biotech and pharmaceutical industries.

These lecture notes is a collection of simulations used by Plant Design group while teaching master students.

Contents

Chapter 1

Thermochemical processes

1.1 Production of synthetic gas from a biomass

The task is to simulate a production of synthetic gas from a 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 is separated. In the simulation, the gasifier is in steady state, isothermal, and decomposition products are estimated based on the biomass ultimate analysis. Tars are not considered in the model, but ashes are taken into account as non-conventional solids. The biomass is the pine sawdust, which is a common waste product of the forest industry. The process flow diagram is presented on figure 1.1.
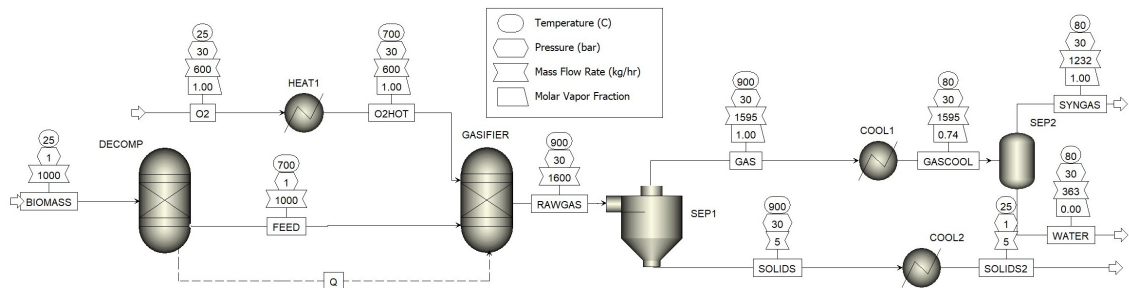

Figure 1.1: Gasification production plant

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 data base 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 "Method/NC Props" tab. The biomass and the ash properties can be estimated by HCOALGEN and DCOALIGT models. 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		
H2	Conventional	HYDROGEN	H2
O2	Conventional	OXYGEN	O2
N2	Conventional	NITROGEN	N2
CO	Conventional	CARBON-MONOXIDE	CO
CO2	Conventional	CARBON-DIOXIDE	CO2
METHA-01	Conventional	METHANE	CH4
CARBOGRA	Solid	CARBON-GRAPHITE	C
S	Conventional	SULFUR	S
H2S	Conventional	HYDROGEN-SULFIDE	H2S
H3N	Conventional	AMMONIA	H3N

Table 1.1: Simulation component

as ULTANAL in Aspen Plus), and sulfur analysis results (denoted as SULFANAL in Aspen Plus). The proximate analysis gives the weight content of moisture, fixed carbon, volatile matter and ash. 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 three types, pyritic, sulfate, and organic sulfur. The DCOALIGT model requires only the two component attributes ULTANAL and SULFANAL. In Aspen Plus it is 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 case of biomass the codes [6 1 1 1], which means that the heat of combustion will be specified. The heat of combustion can be introduced by implementing a new non-conventional parameter in section "Pure Components". Choose the biomass from the list and select HCMOB option to introduce value $18.4[MJ/kg]$.

As there is multiple parameters which needs to evaluated, select option "Estimate all missing parameters" from "Estimation" tab.

Each simulation start from defining an inlet streams. Specify the biomass feed to be 1000[kg/h] at 25°C] and 1[bar]. Enter its Component attribute given 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, as well as the ash present in the biomass. The presence of non-conventional components in the simulation need 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 decompose 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 to consider is the gasifier (presented on figure 1.2). For that purpose let's use the Gibbs Reactor will simply produce an outlet in which the Gibbs free energy of the mixture is minimized. A reaction set can be attached to this reactor, but it is important to note that any parameters specified in the set will not be included in the simulation as the minimization of free energy will be the dominant

simulation 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 oxidizing 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 separation part of the simulation the solids are separated from the hot gases in SEP1, which is an Aspen SSplit. The SS-PLIT assumes perfect separation of solid particles from the main stream. The SEP2 column is a flash column used to separate the condensate. For this the gases is 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 need to be further purified in a separate purification facility to be useful feedstock for other processes.

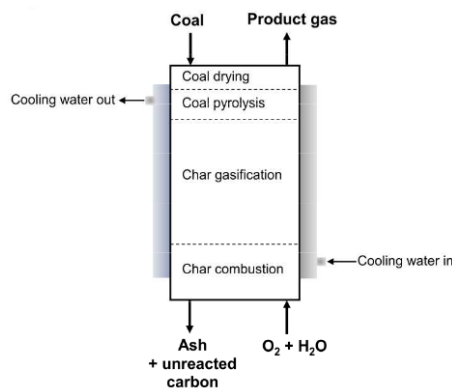The configuration of the simulation and its results are presented below:

	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 are identified in pyrolysis oil and their share depends on the feedstock, process parameters and on the measurement equipment. Therefore, modelling of biomass fast pyrolysis is not trivial. The following assumptions will allow modelling of biomass fast pyrolysis:

- Biomass, ash, char and lignin are define as non-conventional component (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 user defines the pyrolysis products.

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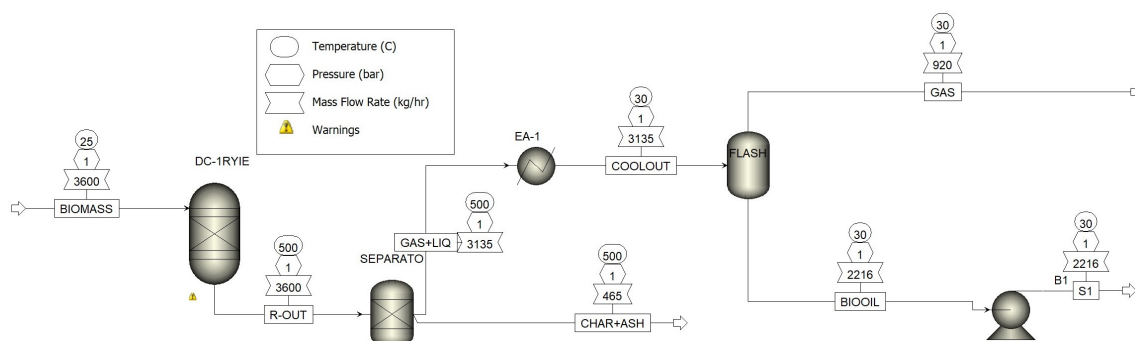

Figure 1.4: Fast pyrolysis plant

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), which is an activity coefficient model used in description of phase equilibria The model is a so-called lattice model and has been 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 from the local composition around another type of molecule. The UNIQUAC model also serves as the basis of the development of 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-acryonitrile and formaldehyde-DMF.

The properties of the non-conventional components need to define. To do so by introducing default values for HCOALGEN and DCOALLIGT.

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)

In the Simulation section, Main Flowsheet, select a yield reactor and connect IN and Out streams. In the Setup sheet, set Stream class to 'MIXNC'. This will enable 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, 1bar and 1kg/s. Use Component Attribute given in table 1.6a. The biomass strem enters the yield reactor which represent the pyrolysis unit. The reaction works at 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 products compositions should be included in "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 main stream. Then the mixture of gaseous and liquid products enter the heat exchanger, which work at $30[°C]$ and $1[bar]$. As the results the condensation occurs. The following step is to separate vapour from the liquid phase in the 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], lets analyse the esterification of lactic acid with methanol given by the following chemical reaction

$$\underbrace{CH_3CHOHCOOH}_{Lactic\ Acid} + \underbrace{CH_3OH}_{Methanol} \rightarrow \underbrace{CH_3CHOHCOOCH_3}_{Methyl\ Lactate} + \underbrace{H_2O}_{Water} \qquad (2.1)$$
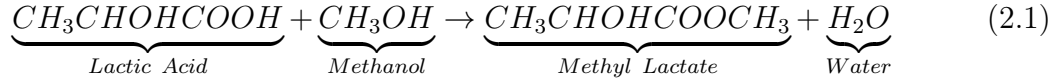
The reaction can autocatalyzed using the acid for temperatures higher than approximately $360K$. The kinetic model is used to represent the reaction rate, but the effect of the reverse reaction is neglected. Thus, the reaction rate is expressed as follows:

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

where k_1 is equal to $6.024 \times 10^8\ [mol \cdot min^{-1}]$, 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 thermodynamic is calculated based on the UNIFAC method. In statistical thermodynamics, the UNIFAC method (UNIQUAC Functional-group Activity Coefficients) is a semi-empirical system for the prediction of non-electrolyte activity in non-ideal mixtures. UNIFAC uses the functional groups present on the molecules that make up the liquid mixture to calculate activity coefficients. By using interactions for each of the functional groups present on the molecules, as well as some binary interaction coefficients, the activity of each of the solutions can be calculated. The UNIFAC correlation attempts to break down the problem of predicting interactions between molecules by describing molecular interactions based upon 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.

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). 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 reactors temperature is determined by the feed 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 in the form of 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 energy of activation E_a are known. The reference temperature T0 is not specified, the exponent n is set as 0 to allow the dependence of temperature to be modeled 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 consider to not efficient enough in terms of the conversion to methyl lactate. The better design can be found by applying the Sensitivity Analysis.

2.2 Heat Exchangers

Let's assume that the reactants don't temperature is not 340[K] as it was specified before, but 293 [K]. To rise the temperature of the inlet stream, a heat exchanger is needed. As the temperature difference is quite 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, that the more precise calculations might be characterised by lower efficiency than the shortcut calculations for example, by taking into account a pressure drop. We use interactive sizing is used to find the heat exchanger geometry. Lucky, there is no error, nevertheless some warnings are present. For simplicity, we are going to modify the simulation to decrease the pressure drop to minimum (0.07 [bar]), as we don't simulate pumps in this work. It is always recommended to check if the pressure drop doesn't force a phase change.

In non-conventional cases, each section of a heat exchanger might be specified by calling a specific TEMA type configuration.

The suggested design is a classic Shell&Tube heat exchanger with one pass. The final result of the heat exchanger design is shown of Figure 2.1.
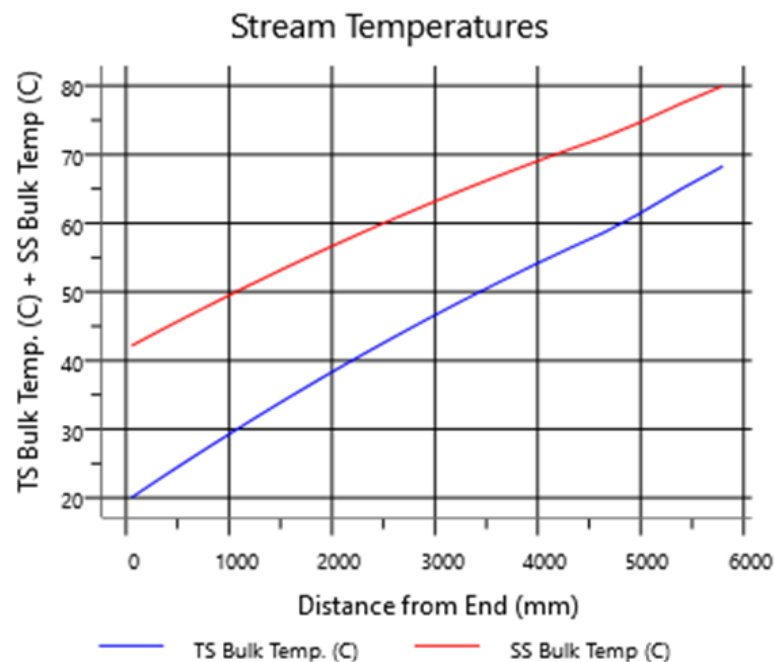
(a) Sensitivity analysis - linear scale
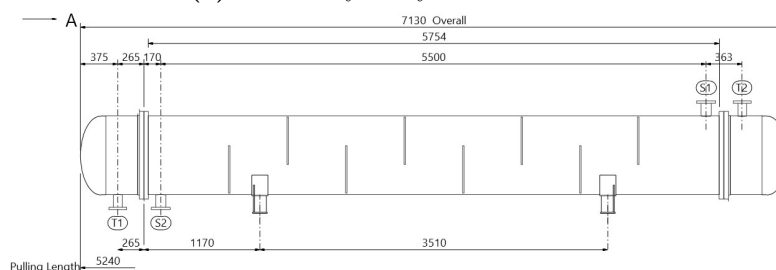
(b) Sensitivity analysis - log scale

Figure 2.1: Sensitivity analysis results

2.3   Sensitivity Analysis

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

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 variable 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, a model output is defined. The model output are affected by a change of 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 result of the sensitivity analysis are present on Figure 2.2.
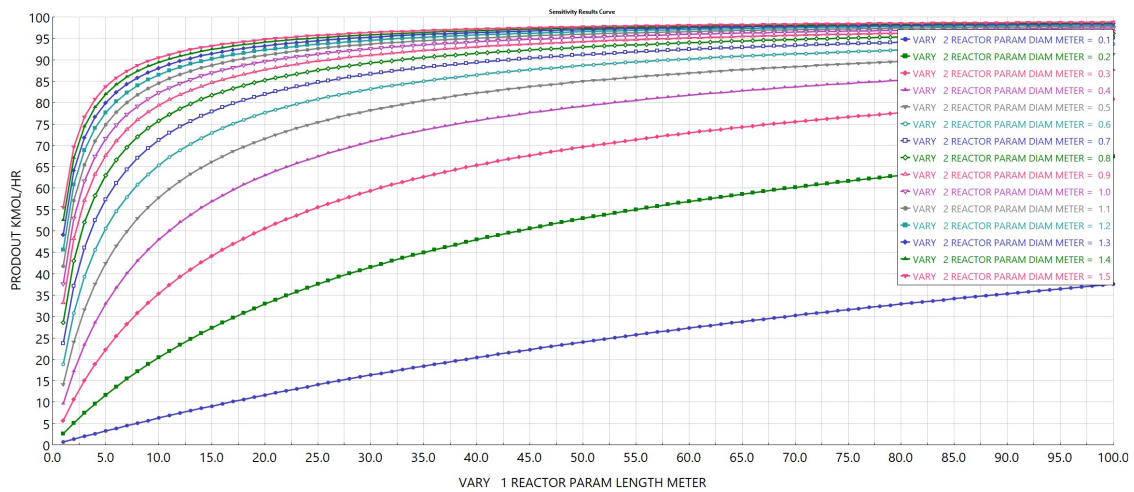
(a) Sensitivity analysis - linear scale
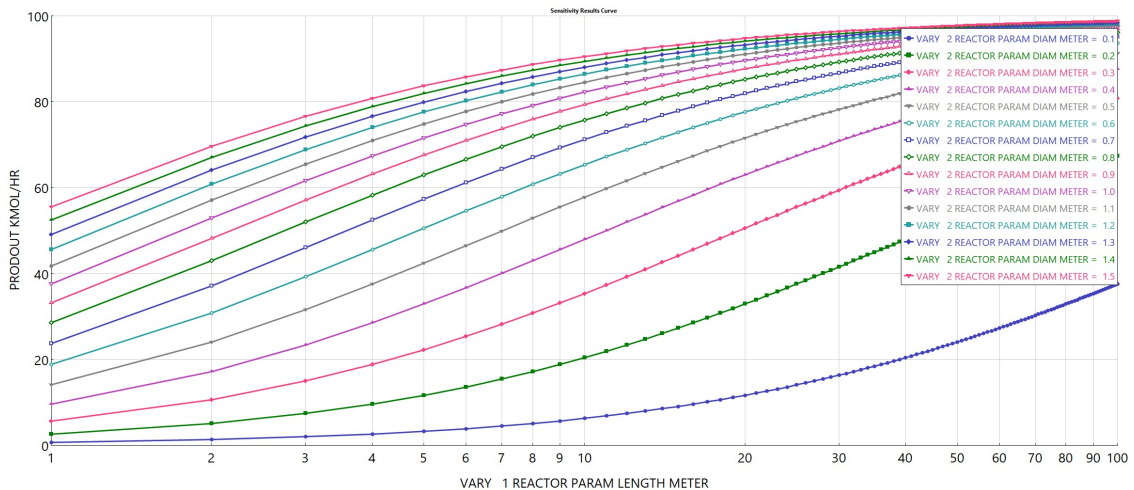
(b) Sensitivity analysis - log scale

Figure 2.2: Sensitivity analysis results

As it is shown on Figure 2.2, the initial value of reactors length and diameter are not sufficient to obtain high conversion.

The next step is to define a local variable, which describe the conversion of lactic acid. Three variables are needs to be defined in the *Define* section. Two variables, which describe the molar flowrate of lactic acid at the inlet and the outlet stream and one which descibe the conversion rate. The molar flowrates can be found in the *Streams* category, as presented above. The conversion is defined as *Local-Param*, but the formula for conversion should be written in the *Fortran* section. Be careful to use the symbols in exact form as they are defined in the *Define* page. The conversion can be calculated from the following equation:

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

The results of sensitivity analysis conducted with respect to the conversion are presented on Figure 2.3.
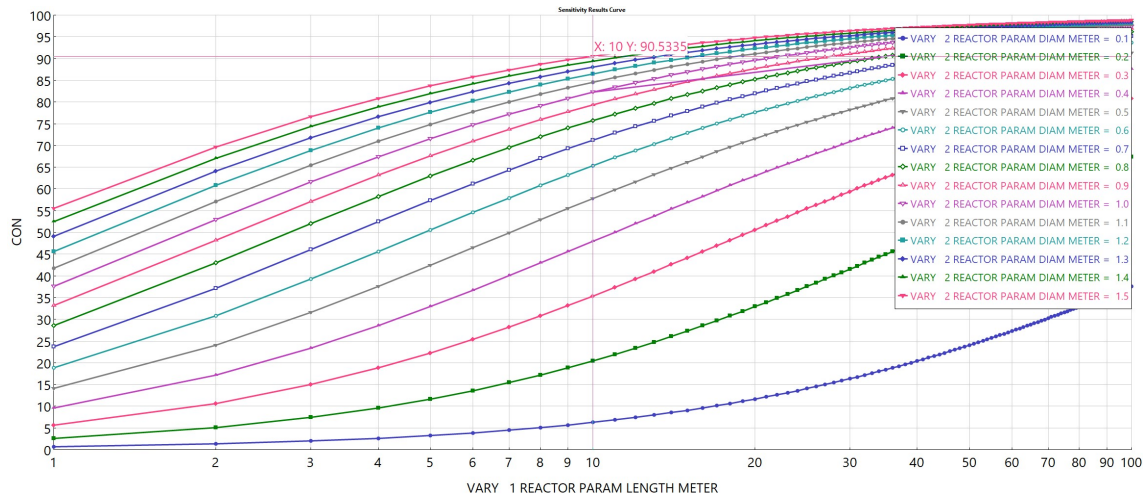
Figure 2.3: Sensitivity analysis with respect to conversion

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

2.4 Design-spec

Lets investigate how to separate compounds of the stream leaving the reactor. By analysis singular points from the Distillation Synthesis Analysis (Table 2.2), it can be notice that there is one azeotrope.

The same conclusion can be drawn form of the ternary plot (Figure 2.4).

	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
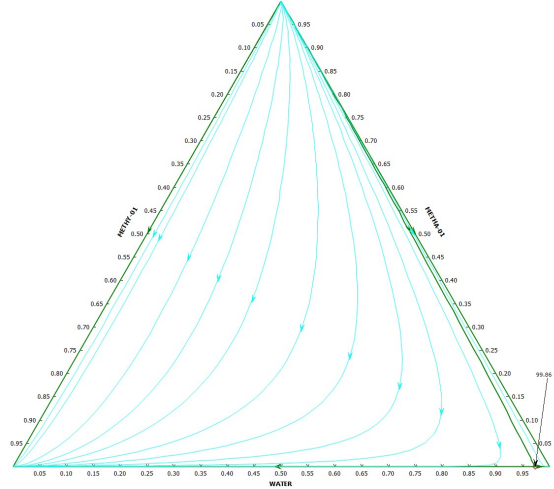
Figure 2.4: Ternary plot

In this simulation work, we are going to remove non-azeotropic components first. We start with *METHA-01*, which is one of reactants and has 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 mole flowrate of the *METHA-01*, and the molar reflux ratio equal 1. To increase the purity of bottom stream, the *Design-spec* is used. 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 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 refulx 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.

2.5   Column Internals

The next step is to analysis the distillation column from the hydraulic point of view. The fact that the simulation of the distillation column has converged and satisfy the mass balance doesn't mean that the hydraulics of the are well designed. This require special attention and separate analysis. The analysis tools for a column hydraulic

		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

can be found in the *Column Internals* folder. One can use the *Auto Section* option to automatically create different sections along the column. In this case, the software suggest two sections of two different diameters (with sieve trays), above and 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 2.5
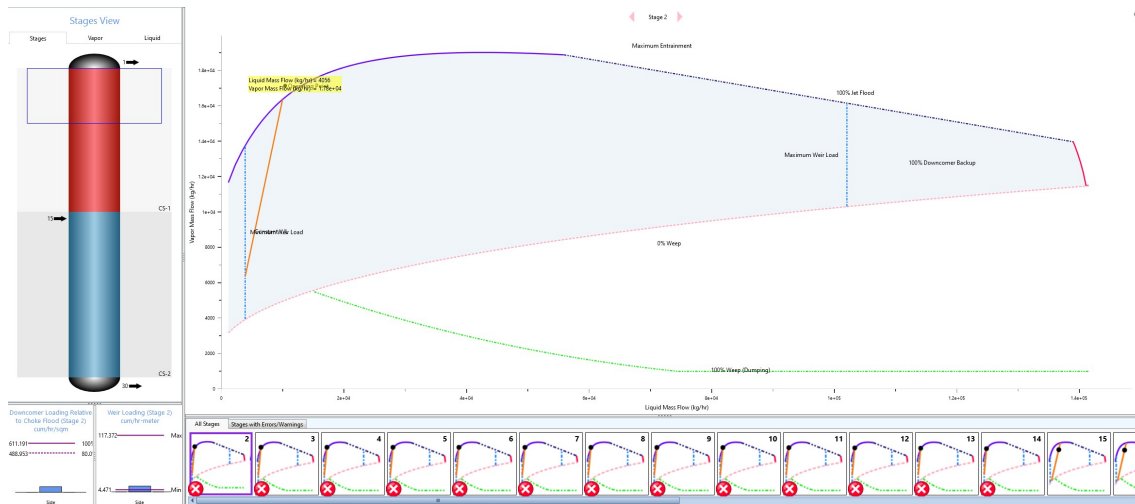
Figure 2.5: Ternary plot

The software return the following error "Entrainments on Stages 2 - 14 are above the specified maximum percent liquid entrainment of 10. We recommend increasing tray spacing." First thing to notice is that both section 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 default value of 0.6096 [m] to 0.75 [m]. The corrected column hydraulic is presented on Figure 2.6.
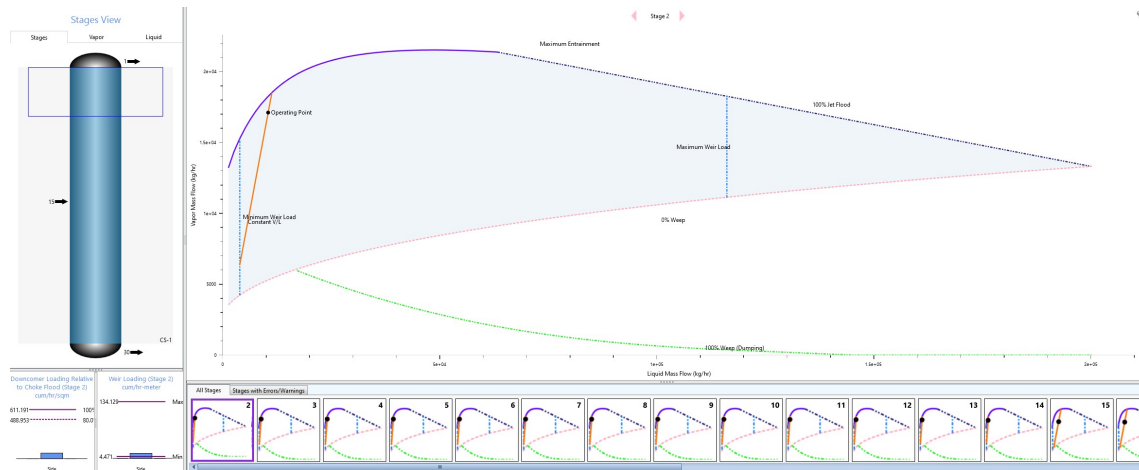
Figure 2.6: Ternary plot

Chapter 3

Economic Analysis

3.1 Acetic anhydride production

To demonstrate how to evaluate the economic attributes of a chemical process, we use the production of acetic anhydride from acetone. 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
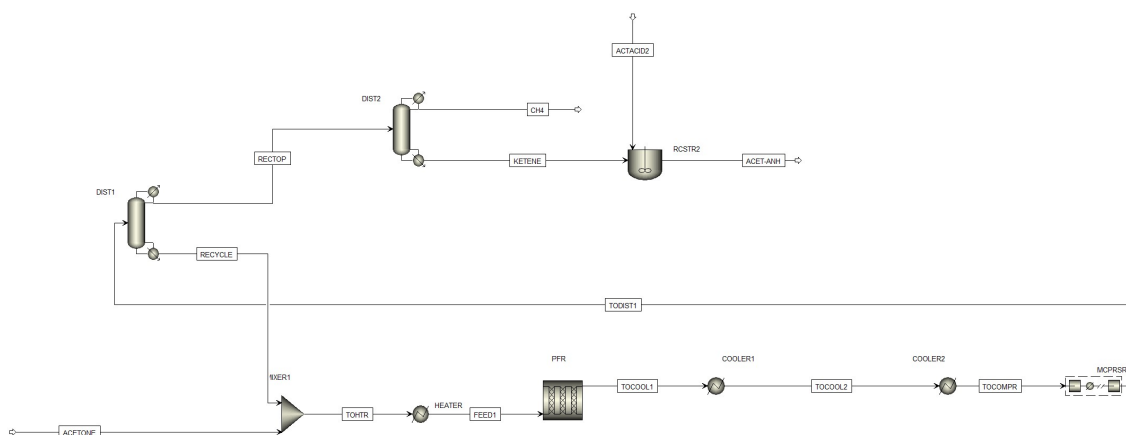
Figure 3.1: The process flowsheet for acetic anhydride production with recycling of the unreacted acetone

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 its 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

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].

Due to the fact that 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 very lower temperature in the condenser. The acetone is a bottom product and is recycled. In the second column, the methane is separated from ketene in a distillation 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 this time 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_3COH_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_3COH_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

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, and defining utilities in terms of pricing and associating them with pieces of 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. If pre-defined utility is used, then it has its own "purchase price" or "energy price". The price of a utility can be

modified by entering detail information of the that utility. The price 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 economic 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 located at the top of the page. The "Size equipment" should be marked, while "Custom sizing" can be left unmarked. "Customize sizing" option allows to interfere with the details of equipment sizing. In the "Map Preview" window all the flowsheet objects are mapped with APEA built-in objects. We are going to used the following mapping:

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

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

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

- Tower type is "Multiple diameter, trayed or packed tower".
- Condenser type is "Bare pipe immersion coil".
- Condenser drum is "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. It

Step 5: Debugging

The next step would be to performed the project evaluation by click on the "Evaluate Project" button. If things go smooth then you will reach the final executive summary for costs without hassles and you can go to the Step 6. However, you may get warning or error messages during the evaluation step regarding sizing or missing input data of some pieces of equipment. f you look at the generated report, you will find that APEA reports an error, which is due to improper entry, such as the type of material of construction or a property value that is out of range. On the other hand, the warning message alarms the user that there might be an error 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 material of construction A214 (Carbon Steel) is not suitable for a high-temperature heater. 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 equipment. After change the inner "Evaluate" button can be used evaluate only the 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 construction for both tube and shell.

Step 6: Project evaluation

Clicking on "Capital Costs" o generate a full-fledge report s that include 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.

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

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

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

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

Step 7: Investment analysis

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 an 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 on figure 3.2.
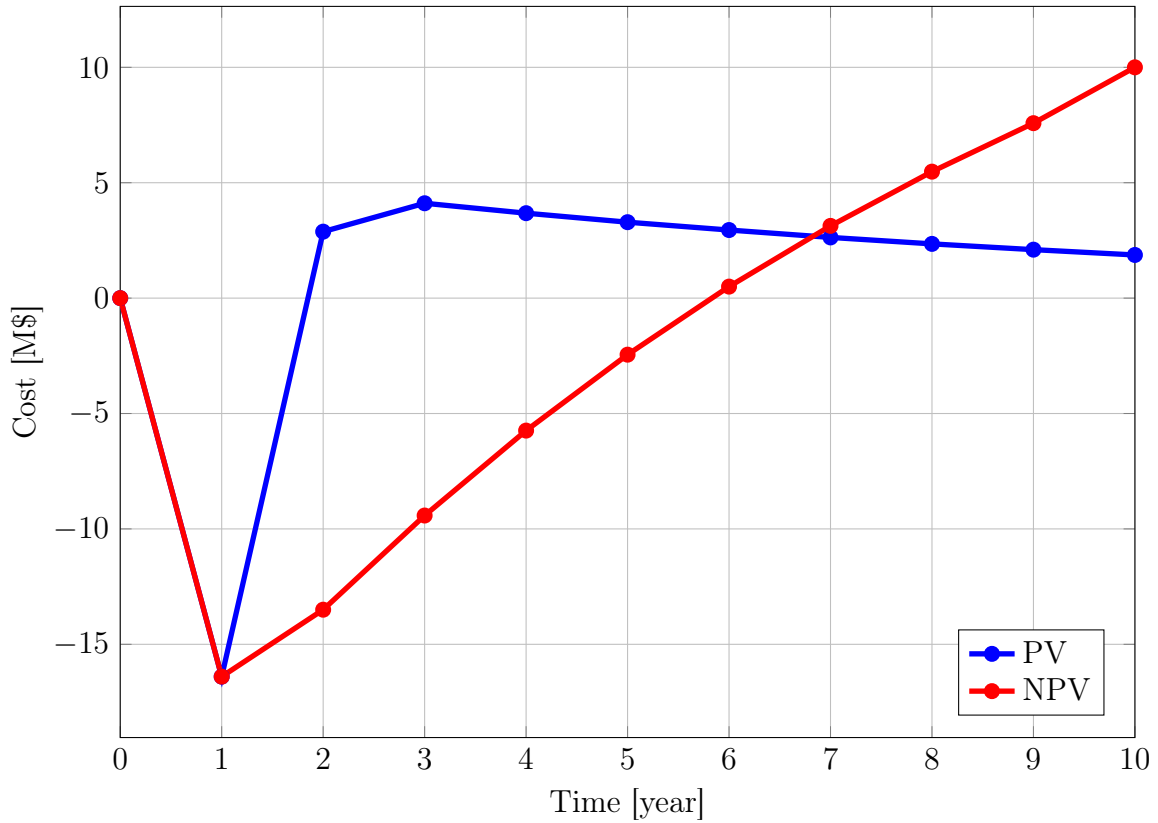
Figure 3.2: Cash flow

NPV is negative for the first 6 years and becomes positive after that, which means that the project appears to be profitable, from year seven onward.

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

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

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

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

If the profitability index is greater than one, then the project appears to be profitable. If this index is less than one, then the project appears not to be profitable. If this number equals one then the project incurs no losses or gains (break-even point). The time evolution of PI is shown on figure 3.3.
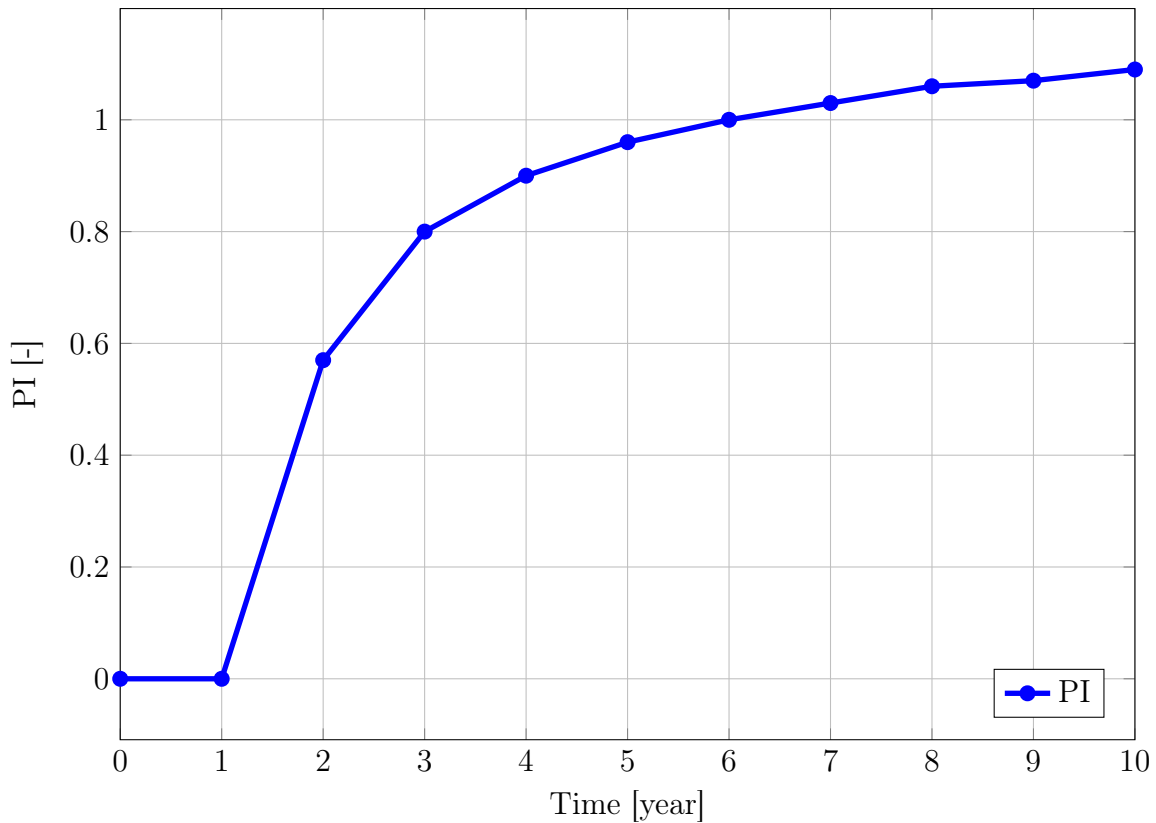

Figure 3.3: Profitability index

The fourth indicator is the **internal rate of return (IRR)**. Iternal 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 that of the investment (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 return on cash. Consequently, if we stick with the assumption of equal rate for both negative and positive cash flow, then IRR gives an optimistic (i.e., overestimated) rate of return for the cash flows. In addition, for projects with alternating positive and negative cash flows, more

than one IRR may be found, which may lead to confusion. To use MIRR, two interest rates are needed: 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.

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

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.

Bibliography

[1] Juan Gabriel Segovia-Hernández and Fernando Israel Gómez-Castro. Stochastic Process Optimization using Aspen Plus®. CRC Press, 2020. ISBN 9780367573096.

[2] Kamal I. M. Al-Malah. Aspen Plus Chemical Engineering Applications. Wiley & Sons, Incorporated, John, 2016. ISBN 9781119293620.

[3] H. Scott Fogler. The elements of chemical kinetics and reactor calculations (a self-paced approach). Prentice-Hall, 1974. ISBN 0132634422.