

MODELLING OF BIOREFINERY PROCESSES

REPORT ON RESULTS & DISCUSSION

By

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Part 1:

1.1 After testing the model with various inputs for validation, here is the methodology along with the assumptions:



Figure 1. Biorefinery Mill Skills



Figure 2. First Excel Mill

Calculations

To calculate the electrical production yield, we have used this equation:

$$Electrical \ yield = mechanical \ yield * 0,95$$
$$Mechanical \ yield = \frac{(HTurbine + MPTurbine + LTurbine) - (P1 + P2)}{Boiler + Reheater}$$

To calculate the heating power produced by each turbine, we have made an energy balance between the entrance and the exits on the turbine.

HP turbine (between (3-4))

$$(Psh + Q)2 = -((q - q1)h4 + q1h4 + q2h4 - qh3)$$

MP turbine (between 5-6):

$$(Psh+Q)5 = -((q3h6) + (q-q1-q2-q3)h6 - (q-q1-q2)h5)$$

LP turbine (between 6-7):

$$(Psh + Q)6 = -(q4h7 - q4h6)$$

The same procedure has been applied to calculate the energy lost in each pump:

Pump one (between 1-2):

$$Psh + Q = out - in = qh2 - qh1$$

Pump two (between 8-9):

$$(Psh + Q)8 = q4h9 - q4h8$$

Boiler 1 (between 2-3):

$$(Psh + Q)2 = qh3 - qh2$$

Reheater (between 4-5):

$$(Psh + Q)4 = (q - q1 - q2) h5 - h4(q - q1 - q2)$$

Table 1. Energy balance calculation

	energy balance between points													
		J	kgars							in	out	out2	out3	k₩
		h	q1	q	q2	q3	q4	q5	q13					psh+fi
point	1	398,0	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000					
	pump 1	-								398,0	411,3	0,0		13,26
point	2	411,3	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000					
	boiler	-								411,3	3422,2			3010,94
point	3	3422,2	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000				q2h4	
	HP									3422,2	2726,8	121,0	0,0	574,42
point	4	2847,8	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000					
	reheater	-								2726,8	3229,2			502,38
point	5	3372,5	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000			q3·h6		
	mturbine									3229,2	3118,6	0,0		110,55
point	6	3257,0	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000					
	LPP									3118,6	2550,5	0,0		568,16
point	7	2663,7	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000					
	condenser	-								2550,5	276,9	0,0		-2273,51
point	8	289,2	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000					
	pump 2	-								289,2	289,3	0,0		0,06
point	9	289,3	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000			in		
	mixer +q1*h4	1								277,0	398,0	121,0		0,00
point	10	398,0	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000			in		
	mixer+q2+q	3								398,0	398,0	0,0		0,00
point	11	356,0	1,0000	0,0425	0,0000	0,0000	0,9575	1,0000	1,0000					

Part 2:

2.1 Study the effect of the preheater outlet temperature (T5) without stream production:

To make this study, we have also made the minimum operating temperature have been calculated as if the reheater won't be adding any heat.

The energy balance in the reheater would be:

$$(Psh + Q)4 = (q - q1) h5 - (q - q1)h4$$

In this case

(Psh + Q)4 = 0

So:

$$(q-q1) h5 = (q-q1)h4$$
$$h5 = h4$$

After having h5 determinate by these conditions, with the XSTEAM you can determinate the minimum temperature needed.

T5 minimum=205,84°C.

So, we have made our calculations between this temperature and the 450 °C which the exercise asked.

It's important to note that for the turbine to operate, the vapor fraction cannot be less than 0.98, which is why T=375 °C is the minimum temperature.

Т5	vapor composition in LPP (xv7)	elec yield (%)	heating power delivered by the condenser
205,84	0,879	32,99	1965
235	0,899	32,86	2011
275	0,924	32,8	2067
300	0,939	32,82	2100
330	0,956	32,89	2138
375	0,9797	33,07	2191
380	0,982	33,09	2197
400	0,9924	33,2	2219
425	1	33,35	2247
450	1	33,52	2274

Table 2. The Effect of Temperature Variation T_5 on the Parameters



Figure 3: Impact of Temperature 5 on Electrical Yield

On the diagram, we can observe two distinct sections: one before the temperature reaches 275°C, and one after. Prior to reaching this temperature, the yield decreases as the temperature increases, while after 275°C, the yield continually improves.

At the critical temperature of 375°C, which is essential for the turbine's functionality, the electrical output is comparable to that of 208°C, the initial temperature where T4 equals T5 in the absence of a reheater. However, this similarity in electrical yield could be attributed to the turbine's insufficient performance, which negatively impacts the overall electrical output. After the T5=375°C it can be observed linear and constant improvement of the electrical yield related to the increasing of the temperature.

The second part of the data pertains to the amount of energy delivered by the condenser.



Figure 4: Impact of Temperature 5 on heating condenser

As the temperature T5 increases, there is a corresponding increase in the energy requirement for the condenser. This indicates that at higher temperatures, more energy is necessary for the process to take place.

Additionally, we can note that it rises in a directly proportional manner.

1.3 Study the effect of varying q3, with q2=0,1 kg/s and T5=375 °C

q3	steam ratio	elec. power production yield	elec. power production yield
0	3,762	30,61%	1968
0,05	2,347	29,87%	1857
0,1	1,683	29,13%	1745
0,15	1,296	28,4%	1634
0,2	1,043	27,63%	1519
0,25	0,866	26,90%	1411
0,3	0,734	26,16%	1299
0,4	0,551	24,68%	1077
0,5	0,43	23,20%	854
0.6	0.344	21.72%	631

Tables 3. Temperature-Parameter Variations Table



Figure 5: Impact of q₃ on Steam ratio

As the steam demand (q3) from the mill increases, the electrical power production yield decreases.



Figure 6. Impact of q_3 on electrical yield

The decline in power generation efficiency becomes apparent as the steam demand ratio rises, demonstrating a negative correlation between these two factors.

Additionally, we can notice that it rises in a direct correlation.

The electricity generation efficiency decreases from approximately 30.61% at q3 value of 0 to about 21.72% at q3 value of 0.6.

The findings indicate that when there is a higher demand for steam in the mill, it has a detrimental effect on the yield of electrical power production. As more steam is redirected, the efficiency of producing electrical power decreases.





It has the same behavior than electrical production yield.

Plot for T5=450 °C :

q3	steam ratio	elec. power production yield	elec. power production yield
0	3,297	30,69%	2042
0,05	2,403	29,89%	1927
0,1	1,705	29,10%	1811
0,15	1,305	28,3%	1695
0,2	1,046	27,51%	1580
0,25	0,864	26,72%	1464
0,3	0,730	25,92%	1348
0,4	0,544	24,34%	1117
0,5	0,422	22,75%	886
0,6	0,335	21,17%	655

Tables 4. q₃-Parameter Variations Table











Figure 10. Impact of q_3 on Heating condenser

In this case we can observe that it has similar behavior in T5=450°C than in T5=375°C, so we decided to compare in the same graphic both values.



Figure 11. Impact of q_3 on Steam ratio



Figure 12. Impact of q₃ on electrical production yield



Figure 13. Impact of q₃ on Heating condenser

Based on the comparison between the values obtained at T5=375°C and T5=450°C, it can be concluded that there is minimal impact on both the energy requirements of the condenser and the output of the mill. However, the increase in either q3 or q2 demand is significant. In this scenario, only the value of q3 has been altered while keeping q2 constant. However, it is believed that increasing the value of q2 would also result in a decrease in electrical output and the energy required by the condenser.

1.4 The optimization strategy involves fine-tuning both back-pressure in the turbines and the outlet reheater temperature (T5) to achieve maximum power production yield in the absence of steam production.

T5=450°C	P4	P6	Electrical yield (%)
	6		32,67
P6=6 bar	9		33,39
	12	6	33,73
	15		33,91
	25		34,07
		2	33,72
P_{4-10} bor	10	4	33,63
P4=10 bar	10	7	33,47
		12	33,25

Table 5. different value of pressure 4

We have made two experiments. Keeping constant P6=6 atm meanwhile we try different values in P4 and the opposite, keeping constant P4=10atm meanwhile we gave different values to P6.

The findings indicate that increasing the temperature of the outlet reheater, while simultaneously reducing back-pressure at turbine P4 and P6, can effectively optimize power generation output when steam production is not a factor.

Part 2

2.1



Figure 14. biorefinery mill cycle with pump 3

In this case, P1 it is increased from 1 bar to 10 bar, so water can increases it's temperature above 100°C without turning into gas. It has also changed the initial temperature from 95°C to 178°C. This fact leads us to choose a new specific pump for the returning flow (q2,q3), in order to facilitate the flow. Without its presence, the fluid will not be able to enter, causing it to reverse its direction.

To do that completely is needed to add a new pump on the 11 flow, because that flux comes to the cycle with a pressure of 1 bar. So, about the new pump we will know that the pressure that goes out is 10 bar, and we already know everything about the flux that comes in (new 12).

Example of how it looks with q2=0,26, q3=0,2 and power/steam ratio=50%

p11	10
T11	85,1
h11,is	356,90558
h11	357,01
s11	1,13
xv11	0
pum	р 3
pum	р 3
pum p12	p 3
pum p12 T12	p 3 1 85
pum p12 T12	p 3 1 85
pum p12 T12 h12	p 3 1 85 355,97915
pum p12 T12 h12 s12	p 3 1 85 355,97915 1,1343591

 Table 7 different parameters of section 11

We have calculated the h11 isentropic with the s12 (that goes inside the pump) and p11 (the pressure after the pump). Afterwards, we used the isentropic after the pump to calculate the actual enthalpy (h11) after the pump and made the new calculations.

$$h11 = h12 + \frac{h12 - h11, is}{pump \ yield}$$

And the new h13, which with the solver will ask it to be equal to h1, it will be calculated making a new energy balance with point 10,11 and 13; out-in=0.

$$q13h13 = q5h10 + (q2 + q3)h11 + Psh + Q$$
$$q13h13 = q5h10 + (q2 + q3)h11 + 0$$
$$h13 = \frac{q5h10 + (q2 + q3)h11}{q13}$$

As we are using mass flow rate, we know that

$$q13 = q5 + q2 + q3$$

This is the way we found the h13 to make the new solver.

To calculate the electrical yield in this point, we added the new pump like this:

$$Mechanical \ yield = \frac{(HTurbine + MPTurbine + LTurbine) - (P1 + P2 + P3)}{Boiler + Reheater}$$

And P3 is the value when you do the energy balance between the point 12 and 11; what goes inside and outside the pump:

$$Pump3 = (q2 + q3) * h11 - (q2 + q3) * h12 = (q2 + q3) * (h11 - h12) = 0,474 kW$$

The results we have obtained:

,	elec yield		power/steam ratio
case a	35,13%	q2=q3=0	/
aaaa b	20 450/	q2=0,26	E10/
case b	30,45%	q3=0,2	51%

Table 8. different value for 2 cases

If both q2 and q3 are zero, it becomes impossible to calculate, however, it yields a mechanical value that is greater than 1 prior to the pump.

When we compare the results both with and without the pump from the first part of the project, we can see that yield increases from 33,25% (without the new pump) to 35,13% (with the pump).

Furthermore, we observed that the electrical yield dropped from 35,13% to 30,45% at a power/steam ratio of 51%, so the electrical yield decreases when we add some q2 and q3 flow, which is quite logical because they will make the machines consume more energy.





By eliminating the pump, we revert to a pressure of one atmosphere, denoted as P=1. Consequently, we introduce an additional reheater within the system, specifically in the turbine section. In this case, the reheater is positioned between the low-pressure (LP) and medium-pressure (MP) turbines, points 6 and 7 in our schema. The new point between 6 and 7, after the new reheater it has been named "62", and it's the flow that goes out of the new reheater and goes in to LP turbine. Flow 6 it is the flow that goes in the new reheater.

		q4h6	ne	w reheater	q4h62				
out mp turbine			in Ip turbine	9			out lp turb	ne	
p6	6	1	p62	5	٦		p7	0.3	
T6	393,481975	q4	T62	450,00			T7	137,57	
h6,is	3244,2					L D turking 00	h7,is	2688,68	
h6	3257,0		h62	3377,67		LP-turbine 90	h7	2757,57	condenser
s6	7,689		s62	7,95			s7	8,12	
xv6	1		xv62	1			xv7	1	

Table 9. Example of how it looks without steam production

To add the new reheater between the MP turbine and the LP turbine, we have calculated the new P like the P that comes out of MP turbine – P lost in the reheater.

2.2.

We have set the temperature on the reheater the same than in point 5, after the first reheater, because we thought that it was the temperature of operation as we did a lot of calculations around it in the first part of this project.

Once we know the pressure and the temperature, the other values have been calculated with the XSTEAM functions on the Excel.

case a	elec yield	31,69%	q2=q3=0
aaaa b	مامم برنماط	26.63%	q2=0,28
case b	elec yield	20,03%	q3=0,2

Table 10. The results we have got in case a and b.

To calculate the electrical yield in this point, we added a new reheater in the electrical yield equation:

$$Mechanical yield = \frac{(HTurbine + MPTurbine + LTurbine) - (P1 + P2)}{Boiler + R1 + R2}$$

R2 is the value when you do the energy balance between the point 12 and 11; what goes inside and outside the pump:

Reheater
$$2 = (q4) * h62 - (q4) * h6 = q4 * (h11 - h12) = 115,5 kW$$

By comparing the results both with and without the reheater from the first phase of the project, we can observe that the yield dropped from 33,25% (without the new reheater, first part of the project) to 31,69% (with the new reheater). The yield decreased, so it is not a good improvement for the project.

Furthermore, we observed that the electrical yield dropped from 31,69% to 26,63% at a power/steam ratio of 51%.

In conclusion, adding a third pump was an excellent idea, but adding a new reheater between the two turbines is not recommended.



Part 3: with pump 3 and with gas turbine heating the reheater

Figure 16. Mill cycle with the gas turbine

Brayton Closed Cycle	Conditions: P1: 100 kPa - T1: P2: 1000 kPa P3: 1150 kPa - T3: P4: 1000 kPa Image: Cold Air Standard (def Execute Clear Output	300 1492.5 ault) Reset F	K K Averag
Cold Air Standard	Cold Air Standard Output		
Cp=1.005 Cv=0.718 k=1.3997214484679665	P1	100	kPa
Initial Values:	T1	300	K
P1 100 kPa	P2	1000	kPa
T1 300 K	T2	579.02	K
P2 1000 kPa	P3	1150	kPa
P3 1150 kPa	T3	1492.5	K
T3 1492.5 K	P4	1000	kPa
P4 1000 kPa	T4	773.29	K
	Pressure Ratio	10	
	Compressor Work	280.41	kJ/kg
	Turbine Work	722.81	kJ/kg
	Back Work Ratio	0.39	
	Heat Input	918.05	kJ/kg
	Heat Output	475.66	kJ/kg
	Cycle Thermal Efficiency	48.19	%

Figure 17.the Brayton Closed Cycle that we have obtained.

Power consumed by the compressor: Compressor Work = 280, 41 kJ/kg air

Specific power produced by the turbine: Turbine work: 7722, 82 kJ/kg air

Specific heat consumed by the burner: Heat output – Heat input = 475,66 - 918,06 = -442,39 kJ/kg air

3.b Calculate the specific enthalpy (kJ/kg) of the flue gas at the reheater inlet

3.1



Figure 18. Specific enthalpy (kJ/kg) of the flue gas at the reheater

To calculate the q air that goes inside the new gas turbine, we had to look on the NIST website the enthalpies of N2 and O2, because we are considering:

$$air \ composition = 20\% * 02 + 80\% * N2$$
$$Q_{reheater} = qmol_{air} \left(0.2 * (h_{in,02} - h_{out,02}) + 0.8 * (h_{in,N2} - h_{out,N2}) \right)$$

As we have been working with mass flow during the project, we will remember that:

$$q_{mol}\left(\frac{mol}{s}\right) = \frac{q_{mass}\left(\frac{Kg}{s}\right)}{M_{air}\left(\frac{kg}{mol}\right)}$$

We are looking for the q_{mass} of air. These are the values that we have obtained in the NIST website:

	hin(500°)	hout(240°)
N2	22,876	14,969
O2	23,613	15,172

Table 11. Values obtained in the NIST website

Q reheater is the result of the balance of energy between the point 4 and 5 in the CHP cycle.

Without steam production, q2=q3=0, we get this value.

Q2=429,44 kW 429,44 = $qmol_{air}(0,2 * (23,613 - 15,172) + 0,8 * (22,876 - 14,969))$ $q_{mol,air} = 53,59 \ kmol/s$

$$q_{mass} = q_{mol,air} * M_{air} = 53,59 * 0,029 = 1,554 kg/s$$

Once we have some value for qair, we can reach to calculate the power delivered by the gas turbine

 $GasTurbine = (Turbine Work - Compressor work) * q_{air} =$

$$= (722,81 - 280,41) \left(\frac{kJ}{kg}\right) * 1,544 \left(\frac{kg}{s}\right) = 683,1 \, kW$$

With this value, you can recalculate the power production yield, putting this inside the mechanical yield and it will be reflected in the electrical yield;

New mec. yield

$$=\frac{(HTurbine + MPTurbine + LTurbine + Gas Turbine) - (P1 + P2 + P3)}{Boiler + R1}$$

And the value obtained after these calculations is electrical yield=56,17 %

To calculate the mechanical yield with steam demand that adjusts itself to power/steam ratio=0,5, we will iterate the value of the power steam ratio=0,5 changing the value of q2 and q3. It is important to mention that the q_{air} needed on the gas turbine will also change.

	without steam	q2=0,35	q2=0,3
	production	q3=0,28	q3=0,35
Q2 reheater (kW)	429,44	254,45	280,96
power/steam ratio	no steam ratio	0,501	0,513
electrical yield (%)	56,31%	31,40%	33,15%
qair turbine (kg/s)	1,554	0,921	1,017
GS turbine (kW)	687,51	407,35	449,79

Table 12. Yield values depending on steam production

About this yield we can observe that without steam production 56,31% > 33,52% (without gas turbine, firsts results). And with stream production 31,40% is not very far away from the original 33,52 without the turbine. We could agree that the gas turbine is a good improvement for the mill. After the economical balance we will know if it is also a good inversion.

To calculate the economical balance, we start looking for the nominal capacity of the gas turbine, then we will determine de annual production. To calculate the annual production, we have guessed a typical value of production hours per year (8760 hours per year)

Nominal capacity
$$GT = q_{air} * (W_{turbine} - BackWorkRatio * W_{compressor})$$

Nominal capacity GT = 1,55 * (722,81 - 0,39 * 280,41) = 953,3 kW

To calculate the annual production of electricity, we will use the next formula:

Anual production
$$(kW) = Nom. Cap. * Elec. Yield_{CHP} * Elec Yield_{GST} * Wk Hours$$

$$Elec Yield_{GST} = Cycle Thermal efficency * 0,95$$

Without steam production an example of calculation would be:

Anual production
$$(kW) = 953,3 * 56,31 * 45,79 * 8760 = 2,15 * 10^{6} \frac{kW}{year}$$

As we know the unit price of electricity sold, we have calculated the income of the CHP cycle without the costs:

Income (without costs) = Anual production
$$\left(\frac{kw}{year}\right) * 0.1 \frac{\notin}{kW} = 2.15 * 10^5 \frac{\notin}{year}$$

The running cost of the turbine is the 90% of this input, so we know that we actually will have 10% of input.

Costs of mantenancy = 2,15 * 10⁵ * 0,9 = 1,94 * 10⁵
$$\frac{€}{year}$$

To do the economic balance of amortization, we made a table on excel

	e	conomic bala	without steam production			
	1st year	2nd year	3rd year	4t year	5th year	6th year
cost investment	70000	0	0	0	0	0
cost manteniment	193930	193930	193930	193930	193930	193930
input electricity	215478	215478	215478	215478	215478	215478
benefits / year	-48452	21548	21548	21548	21548	21548
benefits +	-48452	-26904	-5357	16191	37739	59287

Tables 13. balance of amortization

benefits

$$\frac{\partial energies}{\partial ear} = Total input of electricity - Costs of mantenancy - Costs of turbine$$

So "cost of turbine" will only be 70000 the first year, but the others will already be paid.

For the first year the calculation will be:

$$\frac{benefits}{year} = 215478 - 193930 - 70000 = -48452 \in$$

For the first year, for the second year we will have the still to pay for the negative result, so benefit year will include

$$\frac{benefits}{year} = Total input of electricity - Costs of mantenancy - Costs of turbine + Costs of turbine$$

+Benefits last year =
$$215478 - 193930 - 48452 = -26904 €$$

And it goes on until it is completely paid, which is in this case in year 4. After year 4 you will be obtaining only benefits.

For the case with steam production power steam ratio=0,5 we used the same procedure, and the results are shown in the next table.

	without steam	q2=0,35		
	production	q3=0,28		
nominal capacity (GT) (kW)	953,3	565,0		
hours of work	8760	8760		
Elec Yield Gs (%)	45,78%	45,78%		
electrical yield (%)	56,31%	31,40%		
final elctrical yield is both	25,78%	14,38%		
Anual production of electricity (kW)	2,15E+06	7,11E+05		
steam delivered (q2h4+q3*h6) (kW)	0	1908,7		
Anual production with steam delivered (kW)	2,15E+06	7,13E+05		
unit price of electricity sold euro/kg	0,1	0,1		
income year without costs (euro)	2,15E+05	7,13E+04		
running cost of the gas turbine	90%	90%		
costs mantenancy/year (euro)	1,94E+05	6,42E+04		

Table 14. Results with steam production

Table 15. Economic balance for amortization

	according balance for emertization				q2=0,35					
	economic balance for amortization			q3=0,28						
	1	2	3	4	5	6	7	8	9	10
cost investment	70000	0	0	0	0	0	0	0	0	0
cost manteniment	64211	64211	64211	64211	64211	64211	64211	64211	64211	64211
input electricity	71346	71346	71346	71346	71346	71346	71346	71346	71346	71346
benefits / year	-62865	7135	7135	7135	7135	7135	7135	7135	7135	7135
benefits +	-62865	-55731	-48596	-41462	-34327	-27192	-20058	-12923	-5789	1346

It takes 10 years to amortize it when it has steam flow.

Also, in this case we have added the steam flow to the Annual production steal.

anual production with steam = anual production calculated + steam delivered

After seeing the results on the energy balance we can say that without steam, we wouls start having benefits at the 4th year, with steam we would have to wait the double of time, so depending on the situation it might be a good idea to make the mill work without steam for the 4 first years and after them when the input is only positive and benefits starting the steam demand to the power/steam ratio of 0.5.

As commented before, the yield of the mill it has increased from 33,52% (without pump, without gas turbine) \rightarrow 35,15% (with pump 3, without gas turbine) \rightarrow 56,31% (with pump and gas turbine), so they are good improvements to apply into the mill. We wouldn't apply the new reheater between the MP and LP turbine because it has been calculated that decreases the yield.

We conclude that these two improvements are a good inversion; we will start using the mill until it is paid the turbine without steam demand, 4 years, and then starting to produce demand.