Life Cycle Impact Assessment of Cyclopentanone Production from a biomass and a petrelaic route

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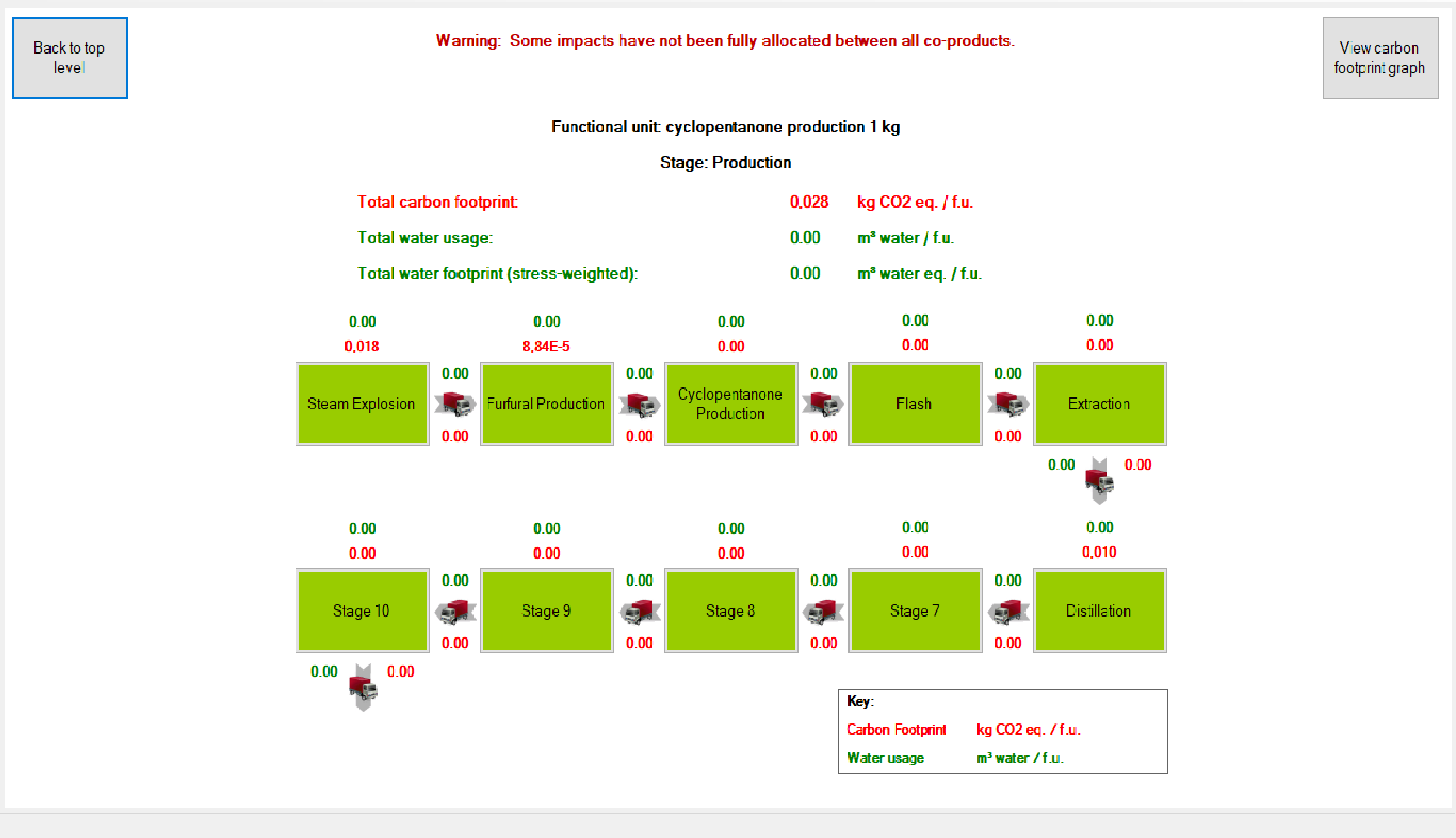
Life Cycle Inventory of Cyclopentanone Production (gate to gate)

Stages	Materials	Input (kg/fu)	Output (kg/fu)
Steam Explosion	Olive Kernels	11.7	
	Xylose		2.03
	Solids (co-prod)		6.18
	Steam (co-prod)		5.70
	CO_2 eq		0.018
	Water	5.85	
	CO_2		2.76
	NO_2		0.048
Furfural Production	Xylose	2.03	
	Furfural		2.03
	CO_2 eq		8.84E-5
Cyclopentanone Production	Hydrogen	0.082	
	Furfural	2.03	
	Cyclopentanone		2.11
Flash	Water (Cooling)	5	
	Cyclopentanone	2.11	2.11
	Hydrogen		0.027

Stages	Materials	Input (kg/fu)	Output (kg/fu)
Extraction	Hexane	0.044	
	Cyclopentanone	2.11	1.21
	COD		0.076
Distillation	Water (Cooling)	9	
	Cyclopentanone	1.21	1
	CO_2 eq		0.01
	COD		3.54
	Furfural (co-prod)		0.00167

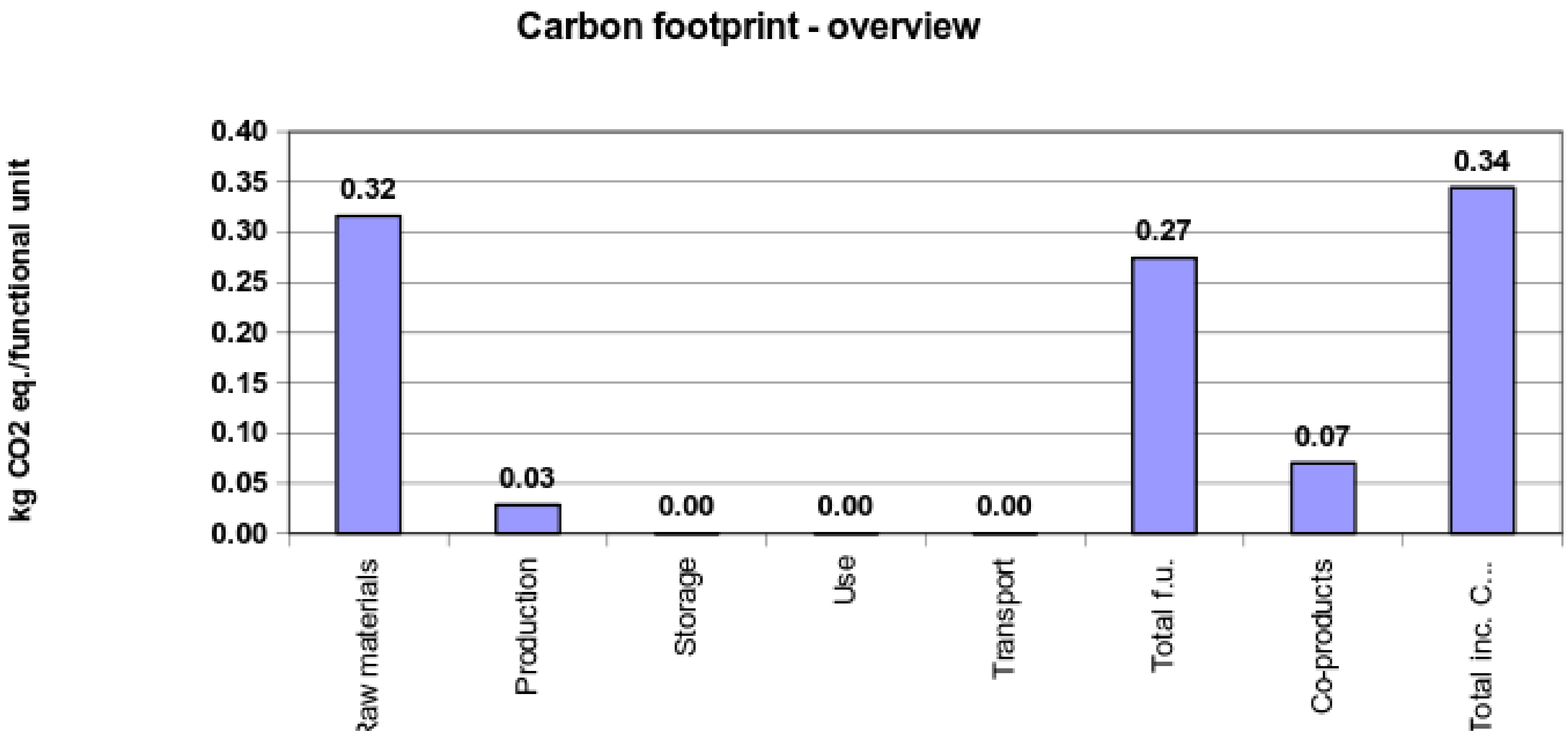
Cyclopentanone Production in CCaLC



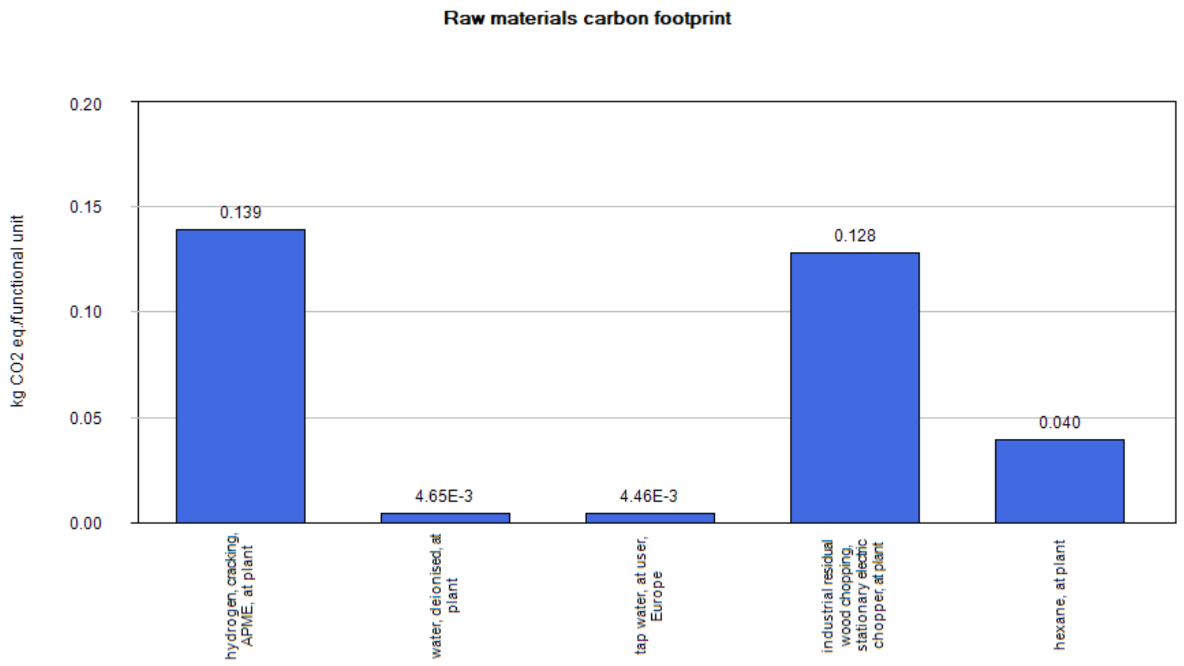
Assumptions for Cyclopentanone Production from Olive Kernels

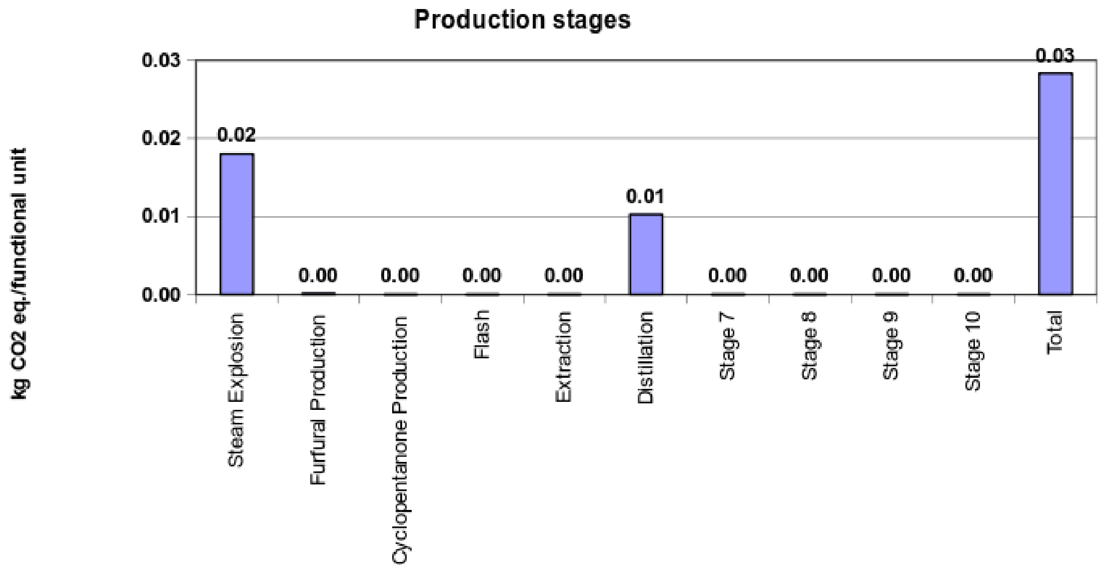
- For the cooling needs it is assumed that regural water is used with no additional energy requirements
- Furfural Production: Xylose $\xrightarrow{\text{Acid Catalysis}}$ Furfural. The acid used is in catalytic amount and wasn't included in the LCI
- The waste streams of the Extraction and Distillation stages are assessed cumulatively as Chemical Oxygen Demand
- The "waste" stream of the Flash stage is considered pure enough in hydrogen to be modeled as a co-product.
- The electricity needed for the pumps is negligible. The electricity needed for the stirring of the CSTRs and other potential needs of the factory were not assessed.
- Olive kernel was modelled as residual wood chopping.
- Heat was modelled as Heat at cogen 1400 kWh, wood as in the original aspen process heat was produced from lignin in a CHP cycle.

Carbon Footprint of the process I

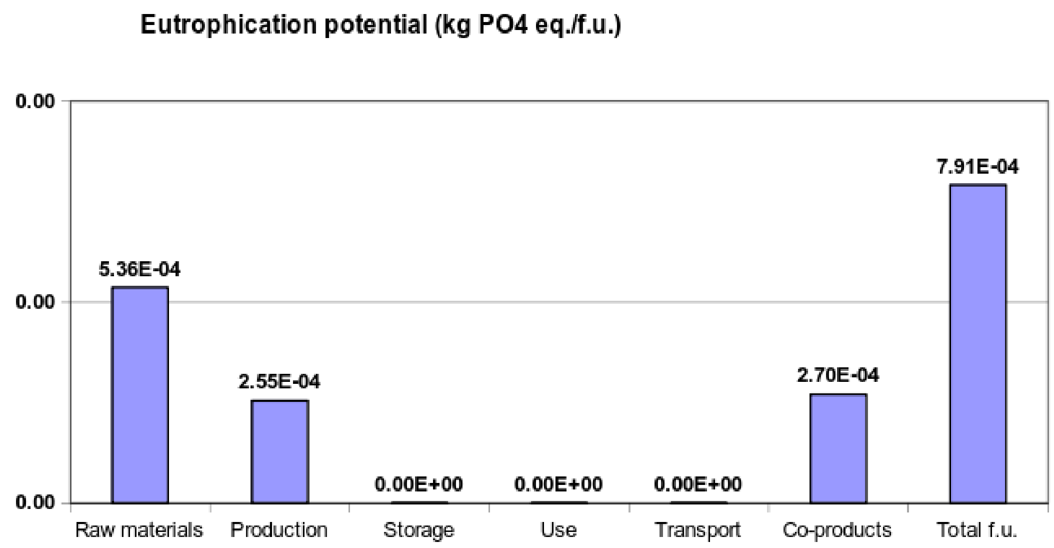


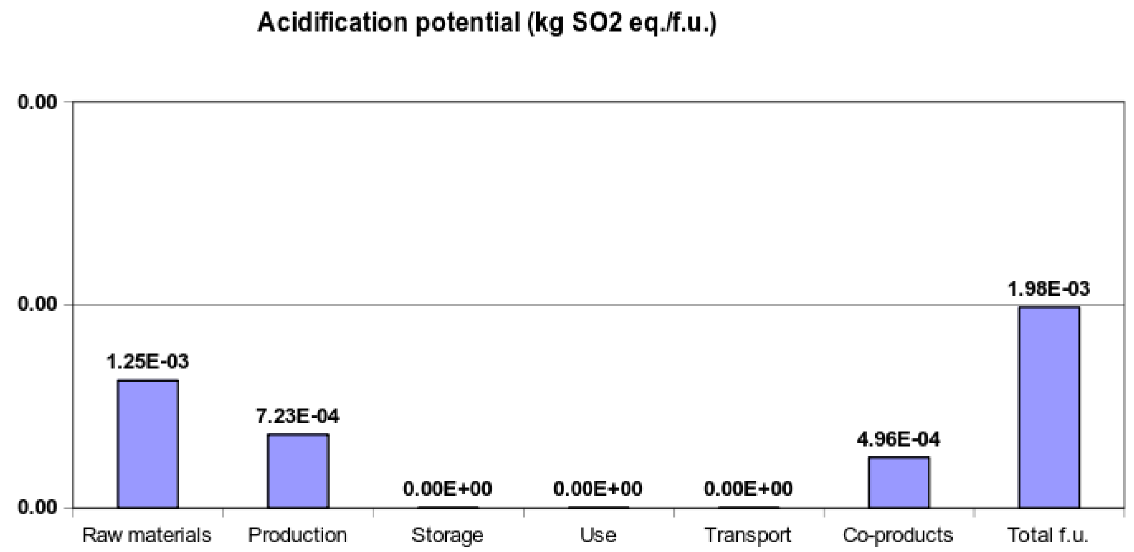
Carbon Footprint of the process II

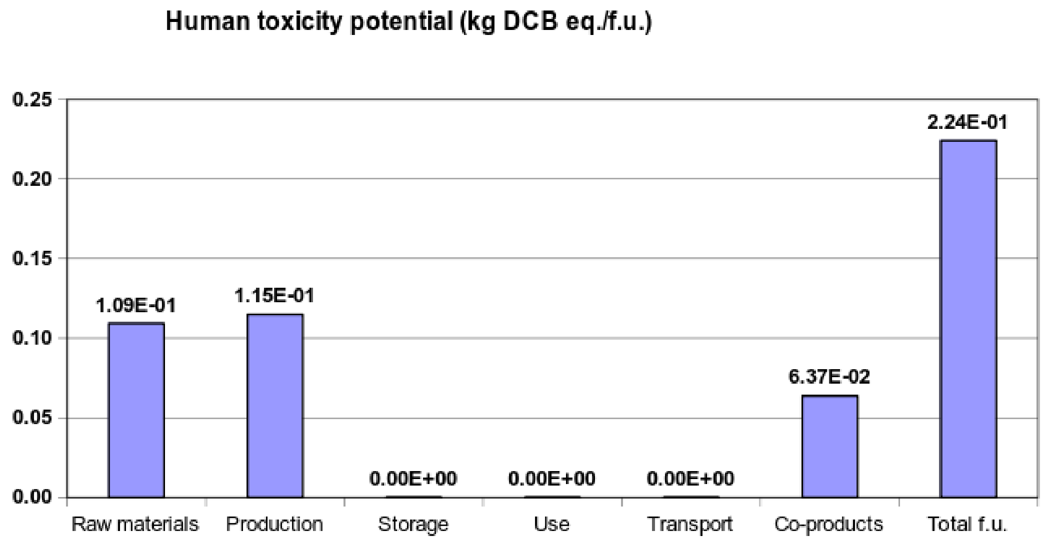


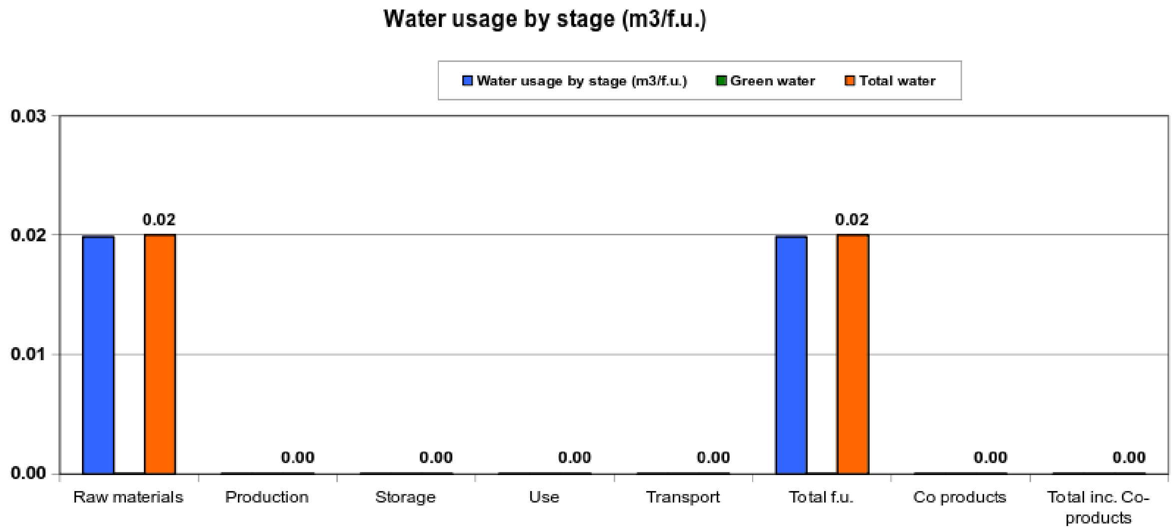


Other Impacts

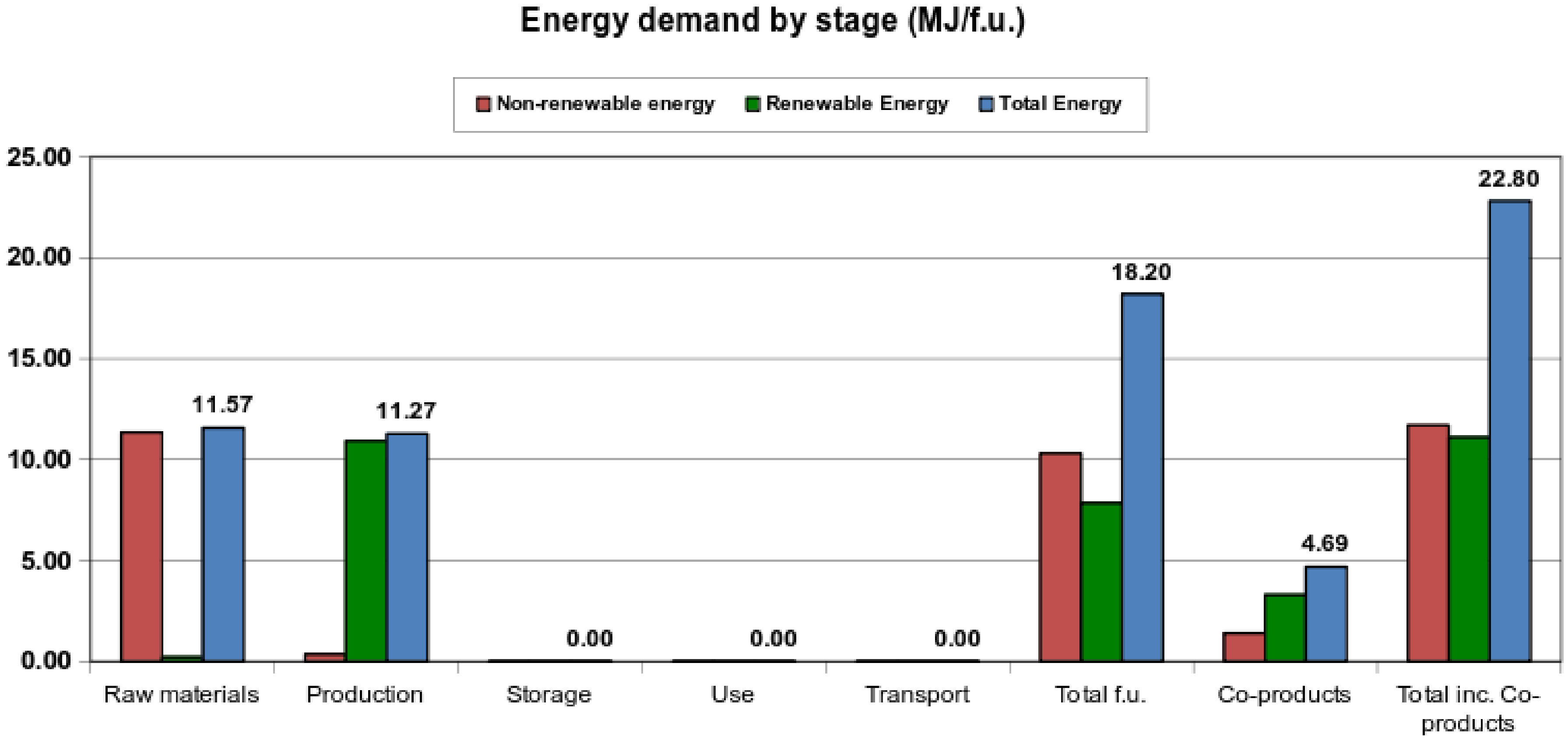








Energy Demand



Process for comparison

We compared our process with a conventional cyclopentanone production process [1], based on petrelaic feedstock and more specifically on the conversion of adipic acid to cyclopentanone when heated with Ba(OH)2 in the mixture.

Ba(OH)2 Production

- Barium hydroxide does not exist in the database used. To assess the environmental impact of the process, data for this is necessary. For this reason, the process was modelled based on a patent describing the production process of barium hydroxide from barite mineral [2].

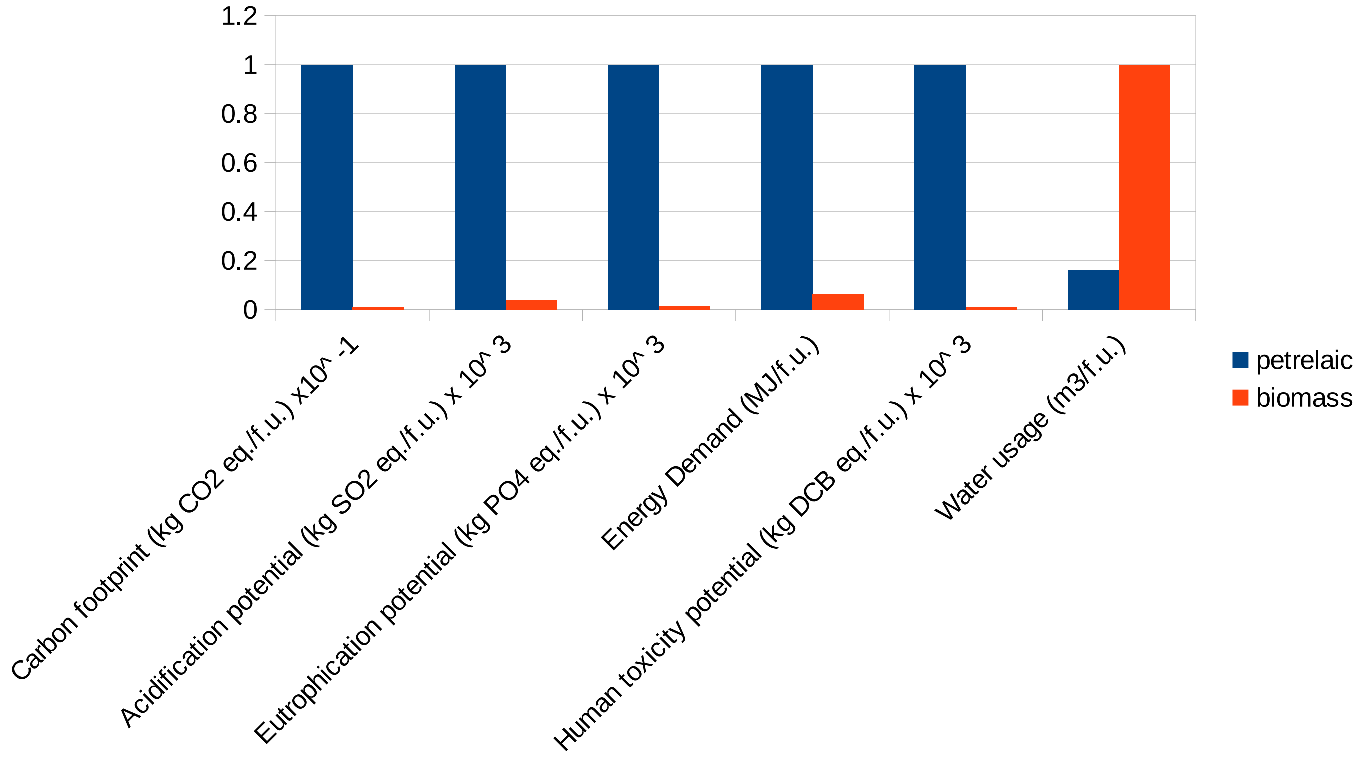
LCI of the process

Raw material	Amount (kg/f.u.)	CO2 eq. (kg/kg raw material)	CO2 eq. (kg/f.u.)	Water usage (m³/kg raw material)	Water usage (m³/f.u.)	Water footprint (stress-weighted) (m³ eq./f.u.)	Database section	Production stage
adipic acid, at plant	2.22	25.4	56.4	0.00	0.00	0.00	Ecoinvent/Ma...	Cyclopentano...
barite, at plant	0.200	0.188	0.038	0.00	0.00	0.00	Ecoinvent/Ma...	Barite Treatm...
compressed air, average inst...	0.140	0.015	2.12E-3	0.00	0.00	0.00	Ecoinvent/Ma...	Aeration Reac...
compressed air, average inst...	2.00E-3	0.015	3.03E-5	0.00	0.00	0.00	Ecoinvent/Ma...	Aeration Reac...
hard coal, at mine, Central an...	0.051	0.250	0.013	0.00	0.00	0.00	Ecoinvent/Ma...	Barite Treatm...
hexane, at plant	0.590	0.900	0.531	0.00	0.00	0.00	Ecoinvent/Ma...	Extraction
water, deionised, at plant	1.22	7.96E-4	9.71E-4	0.00	0.00	0.00	Ecoinvent/Ma...	Leaching
water, deionised, at plant	2.63	7.96E-4	2.09E-3	1.00E-3	2.63E-3	0.00	Ecoinvent/Ma...	Cyclopentano...
water, deionised, at plant	0.122	7.96E-4	9.71E-5	1.00E-3	1.22E-4	0.00	Ecoinvent/Ma...	BaOH crystalli...
Total:	7.18	Total:	57.0	Total:	2.75E-3	0.00		

Energy data: 2 MJ/f.u. heat (modelled as heavy fuel oil), 2.2 MJ/f.u. electricity (electricity mix, Greece), 0.92 MJ/f.u. cooling (water)

Emissions: 0.075 kg CO2/f.u., 0.048 kg SO2/f.u., 2.1 kg COD/f.u.

Comparative LCIA



Conclusion

The conventional process has a very a bad environmental impact due to the existence of adipic acid, whose precursor is benzene. Our proposed process has a much lower environmental impact in every factor besides water usage. Another factor that may affect our process is that it uses the waste material of olive processing and as such, in a cradle to gate approach, it might have an adverse impact in land use. However, this was not assessed at all in our study.

Bibliography

[1] Thorpe, J. F., and G. A. R. Kon. "CYCLOPENTANONE." Organic Syntheses 5 (1925): 37. https://doi.org/10.15227/orgsyn.005.0037.

[2] Rohrborn, Hans-Joachim. Process for producing barium hydroxide. United States US4060585A, filed February 20, 1976, and issued November 29, 1977. https://patents.google.com/patent/US4060585A/en.

Thank you for your attention