



WP4: Integrated design optimisation and LCA – method development and application

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General information



- Open-source, open-access regional optimisation framework implemented as a mixed integer linear program.
- Open-source software has been developed in a Python-based framework, Pyomo with regional data analysis using QGIS.
- The tool is released under the MIT license enabling users to use, modify and redistribute the software and accompanying data in any form.
- The chain tool and accompanying datasets can be accessed through the following link: https://github.com/act-elegancy



Model architecture



For more details, visit WP4 subsection @ https://www.sintef.no/projectweb/elegancy/publications/



How does it work?



An industrial application



- York and the Humber region.
- A population of 5.5 million people.
- Salamanca was built here in 1812 by Matthew Murray.
- Portland cement was invented here in 1824 by Joseph Aspdin.
- Stainless steel was invented here in 1913 by Harry Brearley.
- GVA of £119bn 6.5% of UK.
- Key industries are co-located in this region.



The Humber - emission statistics

- Emissions total ~ 37 MtCO₂ yr⁻¹.
- Regional emissions split heating (14%), process (21%), and power generation (65%) emissions.
- Emissions point concentration of CO₂ vary between 10 30 mol% depending on the asset and its operations.





Key CO₂ abatement options?

Post combustion CO₂ capture

- Requires, ducts, fans and pumps
- Absorber and stripper requirements
- Requires new on-site processes and workforce
- Additional flue gas desulfurisation units
- Additional CHP plant, cooling water tower, etc.

H₂ with CCS

- Additional ATR plant with integrated CCS
- Requires additional piping
- Plant can be located elsewhere
- Furnace and equipment retrofits/ replacements
- Singular point source emission stack



Optimisation superstructure





Core modelling assumptions

- Natural gas is assumed to be available across the region at £13/ MWh. The emissions
 intensity of natural gas is assumed to be 225 g CO₂/ kWh.
- Economic lifetime of 25 years and a cost of capital of 11% is used.
- Demand for heat is assumed to be time invariant across an annual timeframe with 90% availability of the processes.

Modelling overview



- Given the distribution of heat, process and power generation emissions, optimise for the least cost network for net-zero CO₂ emissions in the Humber region.
- Capital cost evaluation includes H₂ production plants and their accompanying equipment, H₂ pipelines, H₂ furnaces/ boilers, CO₂ capture facility and CHP, CO₂ piping, ducting and injection wells.
- Key outputs are total CapEx and OpEx, annualised costs, material flows, life-cycle impact indicators, equipment sizes and emission offset requirements.



Design statistics

	Optimal design		
Total CapEx (£bn)	18.8		
Annual OpEx (£m/ yr)	2210		
Total annualised costs (£m / yr)	4440		
Additional natural gas requirement (TWh/ yr)	65.4		
CO ₂ stored (Mt/ yr)	43.2		
CO ₂ avoided (Mt/ yr)	37.2		
Emission offsets (Mt/ yr)	4.2		
ATR operating capacity (GW)	2		
Post-combustion operating capacity (Mt/ yr)	37.3		
Overall cost of CO_2 avoidance (£/ ton)	119		



CAPEX breakdown - £18.8bn





Life Cycle Impact Assessment

Indicator	Unit	x ⁰
Climate change	Mt CO ₂ eq	2.4
Freshwater and terrestrial acidification	Mmol H⁺ _{eq}	37.7
Freshwater ecotoxicity	GCTU	2.54
Marine eutrophication	kt N _{2,eq}	6.22
Terrestrial eutrophication	Mmol N _{eq}	133
Carcinogenic effects	CTU h	156
Ionising radiation	kt U ²³⁵ eq	438
Non-carcinogenic effects	CTU h	442
Ozone layer depletion	t CFC-11	2.15
Photochemical ozone creation	kt NMVOC _{eq}	20.2
Respiratory effects	unit	307
Fossil use	PJ _{eq}	257
Land use	G unit	17.9
Minerals and metals	t Sb _{en}	42.8

Life Cycle Assessment example: H₂ Production with CCS

- Allows fair benchmarking and identification of trade-offs.
- Life Cycle Inventory (LCI): Datasets with all inputs and outputs related to production of 1 MJ of H₂
- Life Cycle Impact Assessment: Translating all LCI flows into environmental impacts/protection areas: 16 indicators on climate change, ecosystem quality, human health, resources
- The chain tool can do optimisation for these impact categories

For details on the technical and LCA modelling of H_2 production, please see recording and slides from the Work Package 1 Webinar on Monday 21st of June or Antonini, Treyer et al. 2020: Antonini, C., Treyer, K., Streb, A., van der Spek, M., Bauer, C., Mazzotti, M. 2020. Hydrogen production from natural gas and biomethane with carbon capture and storage – A techno-environmental analysis. Sustainable Energy & Fuels, 2020, 4, 2967-2986



Life Cycle Inventories

- Foreground data: All technologies/processes/infrastructure present in the chain tool.
 - Datasets from research within Elegancy or previous research at PSI / literature / databases
 - Datasets adapted where necessary to be consistent with the technological representation in the chain tool (e.g. technical efficiencies, capacity).
 - E.g.: H₂/electricity/heat production, H₂/natural gas boiler, post-combustion CO₂ capture in natural gas power plant, pipelines, storage

Background data

- E.g. input of electricity for production of H₂, input of steel to H₂ production plant
- Ecoinvent v3.6 database transformed into prospective LCI databases representing conditions in 2020, 2030, 2040, 2050
- Reference year for this work: 2020

Producing H₂ and achieving zero or negative emissions

- Contribution analysis shows us where direct and indirect impacts happen
- Carbon-neutral or negative emissions H₂ production possible with both biomethane or wood as feedstock
- Combined with CCS, fossil-based hydrogen («blue hydrogen») is low-carbon and environmentally competitive with H₂ from electrolysis.
- A **net zero-carbon H**₂ **industry** can potentially be achieved by blue&green H₂ combined with negative emissions through biomethane- or wood based H₂.
- H₂ from electrolysis with renewables:
 - Hydropower: ca. 5-30 g CO₂-eq/MJ
 - Wind power: ca. 2-20 g CO₂-eq/MJ
 - Photovoltaics: ca. 20-50 g CO₂-eq/MJ

ATR: Autothermal Reforming // DFB: Steam-blown dual fluidised bed gasifier // EF: oxy-fired entrained flow gasifier // CCS: Carbon capture and storage

Assessing environmental trade-offs

- CCS generally results in higher impacts in all categories other than climate change
- Woody gasification (oxEF) reaches high carbon removal while performing well in most other impact categories.
- Differences between production pathways seem to be large
- Broader context of H₂ applications needed to judge the importance of these differences

Le	gend	Technology type	Least cost	Least climate impact	Least land use impact	Least ozone layer depletion	Least respiratory effects
	Optimisation	Water electrolysis (MW)	0	0	1,300	1,400	400
	Objective	Autothermal reforming with GHR and CCS (GW)	2	3	3	1	3
	Cost-optimal	Post-combustion CO ₂ capture (Mt/ yr)	35.6	31.2	35.3	37.6	35.3
	LCA-optimal (Mt/ yr)	(Mt/ yr)	5.3	7.5	3.8	3.8	3.8
		Cost of CO ₂ avoidance (£/ton)	119	131	131	131	131

Summary

- The chain tool can optimise the performance of the H₂-CO₂ system over a range of performance metrics, providing clarity to decision-makers.
- The tool has included a wide variety of features and technologies through the general-purpose programming framework.
- The tool allows including not only direct environmental impacts, but also indirect impacts from the life cycle chain.
- Model instances can be developed with advanced capabilities to analyse the deployment of infrastructure using various levels of public and private investment.
- The integrated region-specific modelling architecture can be extended to account for other processes and existing infrastructure to develop efficient pathways toward net-zero CO₂ emissions.