Thermo-environomic optimisation of fuel decarbonisation alternative processes for hydrogen and power production

EPFL Thesis (2013): Extended Abstract

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Abstract

To meet the CO_2 reduction targets and to ensure a reliable energy supply, the development and wide scale deployment of cost-competitive innovative low-carbon energy technologies is essential. Switching to renewable resources and CO_2 capture and storage in power plants, are regarded as promising alternatives. To design and evaluate the competitiveness of such complex integrated energy conversion systems, a systematic comparison including thermodynamic, economic and environmental considerations is required. This thesis presents the development of a systematic thermo-environomic optimisation strategy for the consistent modelling, comparison and optimisation of fuel decarbonisation process options. The environmental benefit and the energetic and economic costs of carbon capture are assessed for several process options and energy systems, including H_2 and/or electricity production from natural gas or biomass resources and considering different CO_2 capture technologies. The process performance is systematically compared and the trade-offs are assessed to support decision-making and identify optimal process configurations with regard to the polygeneration of H_2, electricity, heat and captured CO_2.

The results from the systematic process design and comparison studies reveal the importance of process integration, maximising the rational energy recovery by cogeneration, in the synthesis of efficient decarbonisation processes. In addition, the influence of the economic scenario on the process competitiveness and hence on the optimal process design is pointed out. It appears that the various process options are in competition, even with conventional plants without CO_2 capture when a carbon tax is introduced. The choice of the optimal configuration is defined by the production scope and the priorities given to the different thermo-environomic criteria.

Keywords: CO_2 capture and storage, hydrogen, biomass, power plant, process design, process modelling, energy integration, multi-objective optimisation.

1 Problem statement

To meet the challenges of climate change mitigation and sustainable energy supply, several proposals have been investigated, particularly since the Kyoto Protocol in 1997, such as reducing the energy consumption, improving the energy efficiency, changing to less carbon intensive fuels and finally switching to renewable fuels. In the short to medium term, CO_2 emissions reduction by carbon capture and storage (CCS), is considered as a promising option for power plants applications. Three major concepts can be distinguished for CO_2 capture: post-, pre- and oxyfuel-combustion (Metz et al. (2005)). Potential technologies for separating the CO_2 from the other gases are chemical absorption, phsical ab- and adsorption and membrane processes (Figueroa et al. (2008), Kanniche et al. (2010), Olajire (2010), Radgen et al. (2005)). In predictions for post 2020 scenarios (European Commission (2011), Finkenrath (2011), ZEP (2012)), CCS is regarded as cost-competitive compared to other low-carbon alternatives including wind and solar power. The thermo-economic competitiveness of the different CO_2 capture options depends however on the power cycle, the resources, the capture technology and the economic scenario. CO_2 capture reduces the environmental impact on the one hand but on the other hand the power generation efficiency is decreased by up to 10%-points and the production costs are increased by over 30% due to the additional energy requirement and equipment costs for CO_2 capture and compression. Several studies have investigated the penalty of CO_2 capture in terms of efficiency and costs (Figueroa et al. (2008), Finkenrath (2011), Metz et al. (2005), ZEP (2011)). By applying process modelling and simulations, different process configurations for producing H_2 and/or electricity have been evaluated in Berstad et al. (2011), Cormos et al. (2011), Davison et al. (2010), Kvamsdal et al. (2007) and Rosen and Scott (1998). These studies mainly focus on the thermodynamic performance without including detailed heat and power integration. Economic aspects are considered in Kanniche et al. (2010) and Bartels et al. (2010), whereas environmental aspects are taken into account by Viebahn et al. (2007) and Dufour et al. (2012). None of these studies combines extensive flowsheeting with thermodynamic, economic and environmental considerations simultaneously to make a comprehensive comparison of CO_2 capture options in H_2 and power production applications.

To overcome the difficulties of comparing processes with regard to multiple criteria and different assumptions, the goal of this thesis is to propose a comprehensive comparison framework for the quantitative and consistent comparison and optimisation of process options. The objective is to develop and apply a uniform methodology for the systematic comparison and optimisation of different fuel decarbonisation process configurations. By combining thermo-economic models, energy integration techniques, and economic and environmental performance evaluations simultaneously, the platform based on computer-aided tools will support the decision-making process for H_2 and fuel decarbonisation process development, design and operation with regard to several criteria. Special interest is given to the effect of polygeneration of H_2 fuel, captured CO_2, heat and power, in order to identify its advantages and constraints. Through multi-objective optimisation the trade-off between efficiency, CO_2 capture rate and costs is assessed. The potential process improvement of CO_2 capture process integration by internal heat recovery and valorisation of waste heat for combined heat and power generation is investigated. Taking into account the sensitivity of the economic performance to the carbon tax, resource price, operating time, investment and interest rate, it is studied how the optimal process design is influenced by the economic scenario.

1.1 Thermo-environomic optimisation methodology

The process design methodology combines process modelling, using established flowsheeting tools, and process integration models in a multi-objective optimisation framework following the approach presented in Gassner and Maréchal (2009), Gerber et al. (2011) and Tock and Maréchal (2012d). The main features of the methodology are summarised in Figure 1. Technology models representing the physical behaviour are separated from the thermo-economic analysis models and the multi-objective optimisation including energy integration, economic evaluation and environmental impact assessment. Through a MATLAB-language based platform (MathWorks Inc.), structured data is transferred between the different models. The advantage of dissociating the technology models from the analysis models is that process unit models developed with different software can be assembled in a superstructure for subsequent large processes design and optimisation. Moreover, by including the process integration model in the design process the influence of the design and operation is reflected on the thermo-environomic performance of an energy balanced system. First a block flow diagram of the studied conversion process is set up and suitable technologies are summarised in a superstructure, like the one illustrated in Figure 2 for pre-combustion options. For each process unit, chemical and physical models are developed and the heat transfer requirement is defined by using conventional flowsheeting software such as Belsim Vali and Aspen Plus. In the energy integration model, the pinch analysis concept is applied to minimise the energy consumption of the process by calculating thermodynamically feasible energy targets and achieving them by optimising the heat recovery and the combined heat generation. The problem is solved as a Mixed Integer Linear Programming Problem (MILP) minimising the operating costs, while computing the mass balances and the heat cascade as explained in Maréchal and Kalitventzeff (1998) and Gassner and Maréchal (2009). Knowing the flows and operating conditions in the different units of the energy system, the emissions, size and equipment costs are estimated. After having estimated the equipment size by design heuristics, the capital costs of each unit are determined with cost correlations from literature (Turton (2009), Ulrich and Vasudevan (2003)). To evaluate the environmental impacts, life-cycle assessment (LCA) is included in the thermo-economic model as described in Gerber et al. (2011). Finally, multi-objective optimisation applying an evolutionary algorithm (Molyneaux et al. (2010)) is performed to assess the trade-off between competing objectives and identify competitive process configurations.

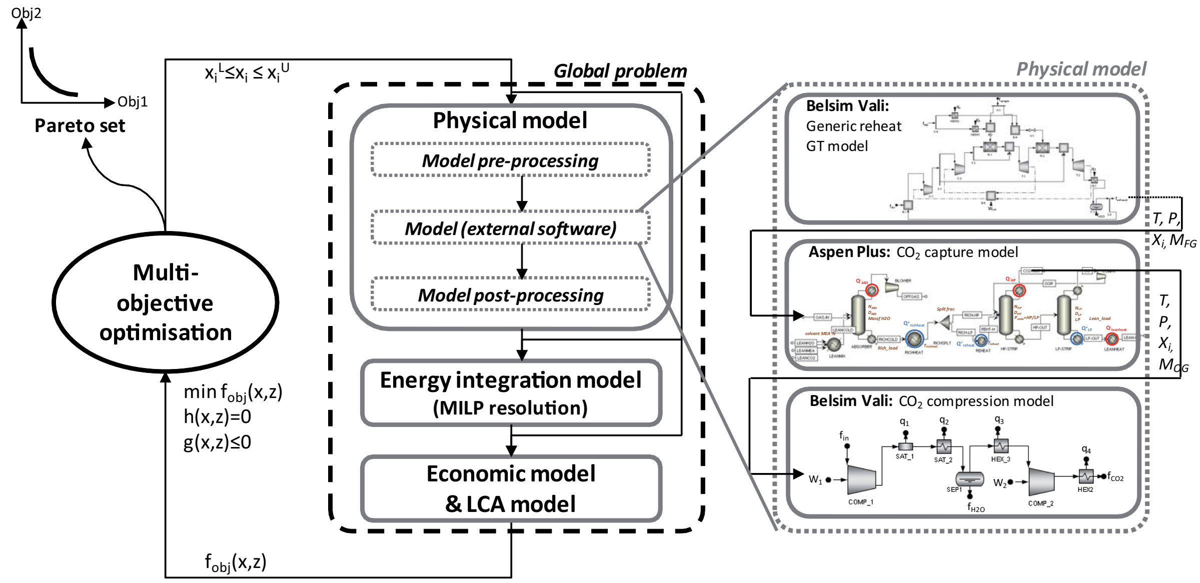


Figure 1: Illustration of the developed platform for studying energy conversion systems.

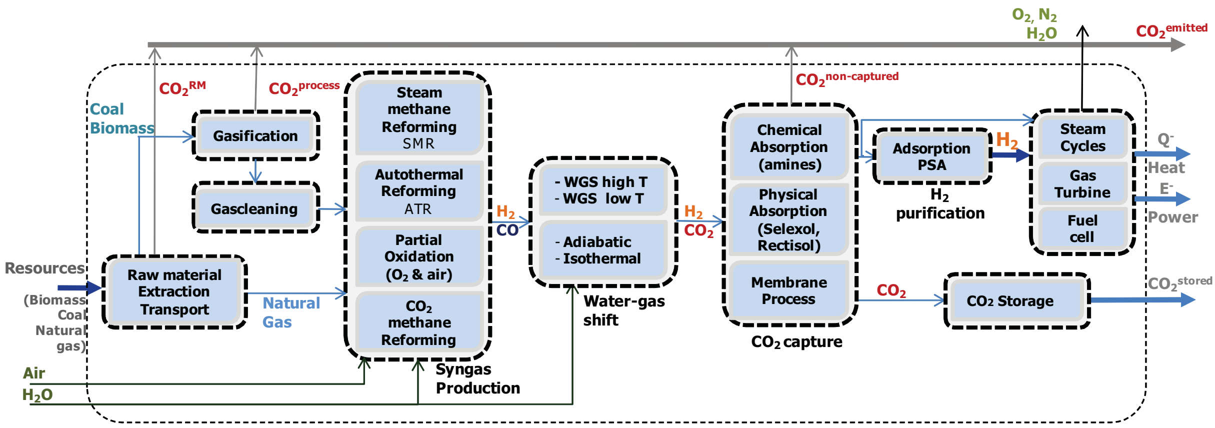


Figure 2: Process superstructure of pre-combustion CO_2 capture process options.

2 Systematic comparison of CO_2 capture options

To assess the impact of the CO_2 capture concept and technology on the competitiveness of H_2 and/or electricity production processes, the different process options illustrated in Figures 2 and 3 are investigated. Natural gas (NG) and biomass (BM) (i.e wood) are considered as a resource. Coal applications have been studied separately in Urech et al. (2013). The captured CO_2 is compressed to 100bar for subsequent transport and storage. It is focused here on the electricity production processes, however CO_2 capture in H_2 production processes has also been assessed. The models and results have been published in Tock and Maréchal (2012a,b), Tock and Maréchal (2012d,e) and Tock and Maréchal (2012c).

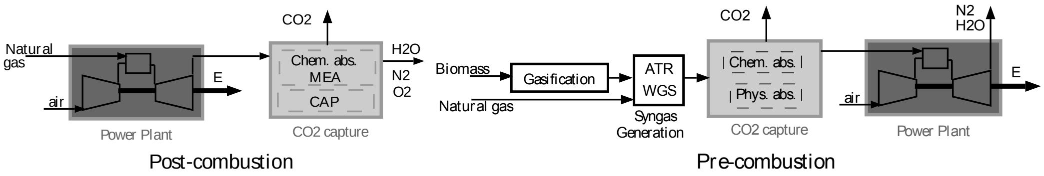


Figure 3: Investigated CO_2 capture options for electricity production.

The competitiveness is evaluated by the energy and cost penalty and the environmental benefit of capturing CO_2 in power plants. The environmental benefit is expressed by the local CO_2 emissions and the overall life cycle impacts assessed for different impact methods for a functional unit of 1GJ of electricity produced. A conventional natural gas combined cycle (NGCC) power plant without CO_2 capture is considered as a reference. The CO_2 avoidance costs $(\frac{COE_{CC}-COE_{ref}}{CO_{2,emit,ref}-CO_{2,emit,CC}})$ are calculated with regard to this reference. The economic performance is evaluated for the economic scenarios defined in Table 2. The energy efficiency and CO_2 capture rate are maximised by multi-objective optimisation. Based on Pareto results, as the ones presented in Figure 4, compromise process configurations with 90% of CO_2 capture are selected for natural gas fed processes and with 60% of capture for biomass processes. The performance results are summarised in Table 1 and Figure 5.

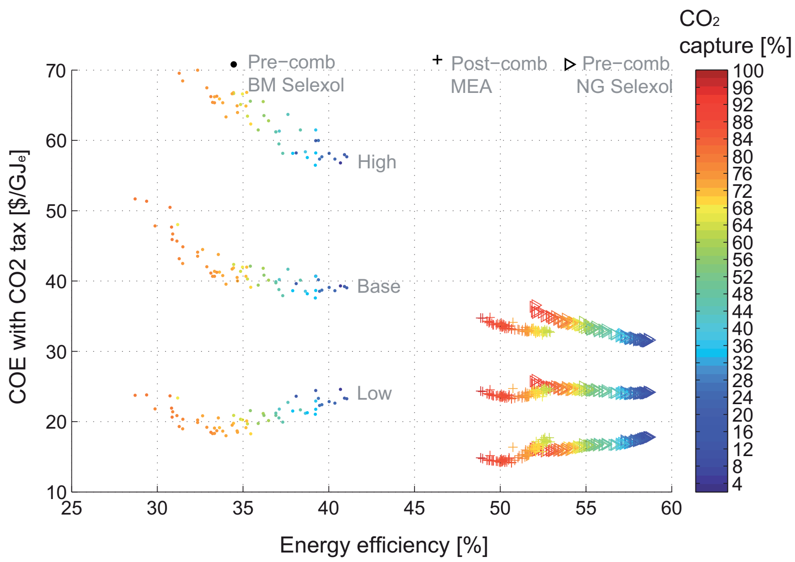


Figure 4: Multi-objective optimisation results: Performance of power plants with CO_2 capture for different economic scenarios reported in Table 2.

Pre-combustion CO_2 capture processes reveal to perform slightly better in terms of energy efficiency than post-combustion CO_2 capture processes. In pre-combustion CO_2 capture processes the energy demand for CO_2 capture is lower, however the capital investment is larger because of the more complex installation. The electricity production costs are hence comparable for both concepts (Figure 8), since the higher productivity compensates the additional investment almost for the pre-combustion CO_2 capture processes. CO_2 capture in biomass fed processes leads to a lower electrical production efficiency and to higher costs due to the limited biomass conversion efficiency and to the high investment costs for the gasification process (Figure 8).

Table 1: Performance of the different power plant options with CO_2 capture.

System Capture technology	NGCC no CC	Post-comb MEA	Post-comb CAP	ATR TEA	ATR Selexol	SMR TEA	BM TEA	BM Selexol
Feed [$MW_{th,NG/BM}$]	559	587	588	725	725	725	380	380
CO_2 capture [%]	0	89.5	89.7	89.7	89.1	89.3	59	59
ϵ_{tot} [%]	58.75	49.6	50.9	56.8	52.6	53.3	34.8	34.8
Power Balance								
Net electricity [MW_e]	328	291	299	408	375	381	132	132
$\dot{E}^{+}_{Consumption}$ [$MJ_e/GJ_{e,net}$]	-	108.3	44	91.9	146.6	48.1	342.4	342.4
$\dot{E}^{-}_{SteamNetwork}$ [$MJ_e/GJ_{e,net}$]	340.7	341.3	301	200	177.6	143.8	346.2	346.2
$\dot{E}^{-}_{GasTurbine}$ [$MJ_e/GJ_{e,net}$]	659.3	767	743	891.9	969	904.3	996.2	996.2
Economic Performance (Assumptions Table 2- Base)								
Invest. [$/$kW_e$]	555	909	785	757	813	798.8	7380	3880
COE no CO_2 tax [$/$GJ_e$]	18.31	23.7	22.5	22.67	24.5	24.1	66.1	49.5
COE with CO_2 tax [$/$GJ_e$]	22	24.2	22.8	23.0	24.9	24.5	60.2	43.6
Avoidance costs [$/$t_{CO2,avoided}$]	-	60	43	46	66	62	173	113
Environmental Performance ($FU=1GJ_e$)								
CO_2 emissions [kg_{CO2}/GJ_e]	105	14.9	8.5	10.1	11.5	11.2	-170.4	-170.4
IPCC GWP [$kg_{CO2,eq}/GJ_e$]	120	34	27.7	30	31.9	36.1	-139.6	-134.2
EI99 [pts/GJ_e]	7.48	7.7	7.7	7.7	8.1	9.0	6.2	6.1
Impact 2002 [$10^{-3}pts/GJ_e$]	28.9	20.8	20.3	21.5	22.4	25	2.9	3.2
CML Acidification [$10^{-2}kg_{SO2,eq}/GJ_e$]	20.1	14.9	15.4	20.6	21.8	24.3	21.3	21.1
CML Eutrophication [10^{-3} $kg_{PO4,eq}/GJ_e$]	39	23.6	24.4	37.7	40.6	43.5	95.1	95

However, these renewable processes have the advantage of capturing biogenic CO_2 and will thus become interesting if a carbon tax is introduced. It has to be noted that the considered biomass plant's capacity of $380MW_{th,BM}$ is much lower than the one of the natural gas plants (580 and $725MW_{th,NG}$). The biomass plant's scale is limited by the biomass availability and the logistics of wood transport, as explained in Gerber et al. (2011).

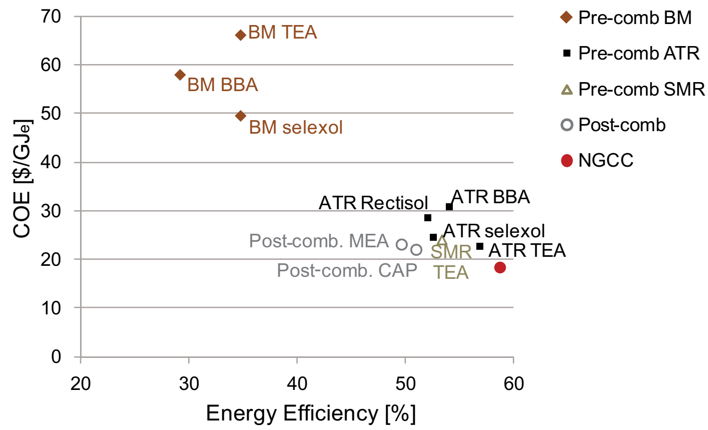


Figure 5: Performance results of the different power plant options with CO_2 capture. For natural gas fed processes a capture rate of 90% is considered and 60% for biomass fed processes (Table 1).

2.0.1 Environmental performance

Life cycle assessment is performed to evaluate the environmental impact of the electricity production ($FU=1GJ_e$). In the life cycle inventory phase every flow, crossing the system boundaries as an extraction or an emission, which is necessary to one of the unit processes, is identified and quantified based on the process layouts. The major process steps are resource extraction, syngas production, gas treatment and CO_2 removal, and heat and power generation. The climate change impact of the different process options is detailed in Figure 6 for the IPCC 2007 method. Compared to a conventional NGCC plant without CO_2 capture, the benefit of capturing CO_2 can clearly been seen. For the natural gas fed processes, the major contributions to the greenhouse gas emissions are coming from the natural gas and from the uncaptured CO_2. With CO_2 capture, the contribution from the natural gas is slightly larger because of the lower power plant efficiency. For biomass fed processes, the advantage of capturing biogenic CO_2 is revealed by the negative overall CO_2 balance.

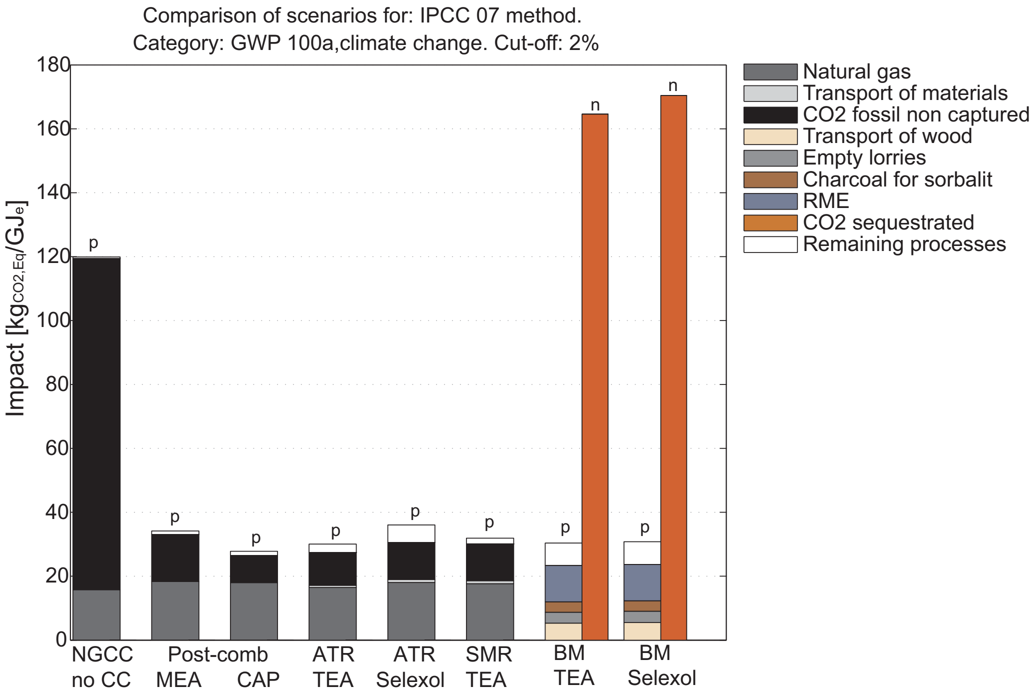
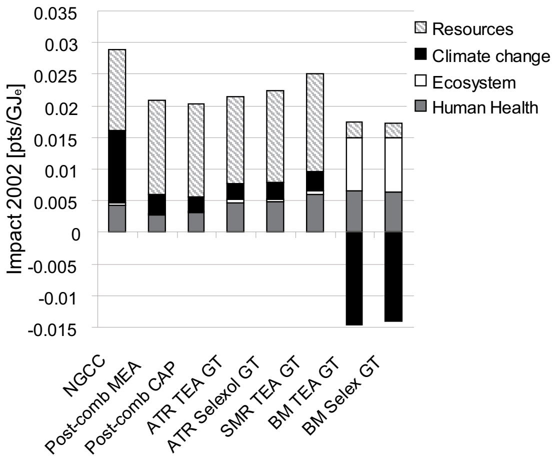


Figure 6: Comparison of the climate change impact of power plants without and with CO_2 capture based on the impact method IPCC 07 for $1GJ_e$. Contributions that are harmful are labelled with a p and beneficial ones with an n.

The damages on the other impact categories assessed with the Impact 2002+ and Ecoindicator 99 method are reported in Figure 7.



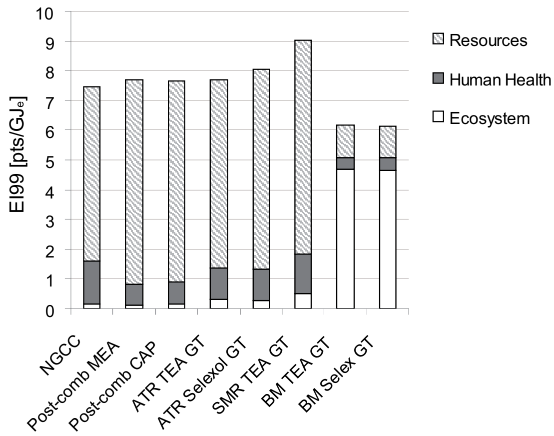


Figure 7: Comparison of the life cycle impacts of power plants without and with CO_2 capture based on the impact methods Impact 2002+ (left) and Ecoindicator 99-(h.a) (right) for $1GJ_e$. Contributions that are harmful are positive and beneficial ones negative.

For natural gas based processes with CO_2 capture, the impact on the resources is large since fossil resources are depleted. Due to the energy demand for CO_2 capture and compression, the natural gas consumption is increased to produce 1 GJ of electricity compared to a conventional plant without CO_2 capture having a higher productivity. For processes using biomass, which is a renewable resource, the impact on the resources is not significant, however the impact on the ecosystem is important. The usage of renewable resources, such as wood, influences of course the ecosystem. The largest contribution is however attributed to rape methyl ester (RME) consumed in the cold gas cleaning step. RME is produced from colza which is cultivated with insecticides. To reduce this impact alternative colza cultivation methods, the usage of other types of oils, and the development of alternative cleaning methods have to be investigated. Using renewable resources to produce ammonia will also considerably reduce the environmental impact as reported in Tock et al. (2012f).

The comparison of the environmental impacts of CO_2 capture in power plants clearly reveals the benefit of reducing greenhouse gas emissions on the climate change. Considering also other environmental impacts, no clear decision in favour of one specific capture concept can be made.

2.0.2 Economic performance

The economic competitiveness of CO_2 capture highly depends on the resource price. In fact, the costs are defined by up to 80% by the resource purchase as shown in Figure 8.

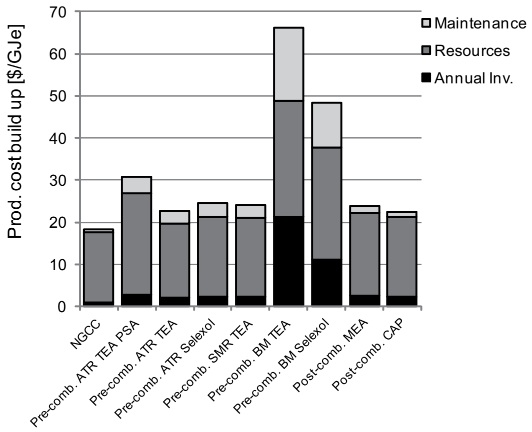


Figure 8: Production cost build-up (Base).

Scenario	Base	High	Low
Resource price [$/GJ$_{res}$]	9.7	14.2	5.5
Carbon tax [$/t$_{CO2}$]	35	20	55
Yearly operation [h/year]	7500	4500	8200
Expected lifetime [years]	25	15	30
Interest rate [%]	6	4	8
Biomass feed [MW$_{(th)}$]	380	380	380
NG feed (post-comb) [MW$_{(th)}$]	725	725	725
NG feed (pre-comb) [MW$_{(th)}$]	590	590	590

Table 2: Definition of the economic scenarios.

The variation of the electricity production costs with the resource purchase price and the introduction of a carbon tax is studied by sensitivity analyses in Figure 9. When a carbon tax of 35$/t$_{CO2}$ is introduced, the economic benefit of a conventional NGCC is reduced and scenarios with 90% of CO_2 capture become competitive (Figure 9 left). The break even natural gas price for which post-combustion CO_2 capture becomes competitive is around 6$/GJ$_{NG}$ for a carbon tax of 35$/t$_{CO2}$. Under the base case economic conditions, the break even carbon tax is around 50$/t$_{CO2}$ for post-combustion capture with MEA and around 62$/t$_{CO2}$ for pre-combustion capture with Selexol as shown in Figure 9 (right). Due to the benefit of capturing biogenic CO_2, CO_2 capture in biomass fed power plants becomes competitive with natural gas fed processes for a carbon tax of 62$/t$_{CO2}$. In these analyses, the CO_2 capture rate and thus the process design are fixed. However, it is evident that there is a trade-off between the economic performance and assumptions, and the process design, in particular the CO_2 capture rate.

3 Conclusions

In the perspective of a sustainable energy future driven by greenhouse gas constraints, CO_2 emissions have to be decreased, energy conversion efficiency has to be increased and fossil resources have to be progressively replaced by renewable resources. For the purpose of designing such complex integrated energy conversion systems and guiding decision-making and development,

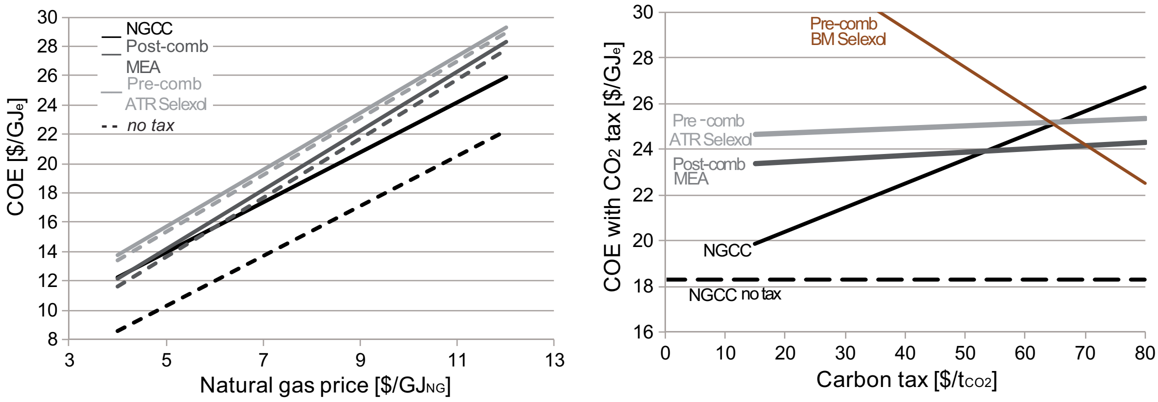


Figure 9: *Left:* Influence of the natural gas purchase price on the electricity production costs without (- -) and with (–) the inclusion of a carbon tax of 35$/$t_{CO2}$. *Right:* Influence of the carbon tax on the electricity production costs without and with CO_2 capture for a natural gas price of 9.7$/$GJ_{NG}$ and a biomass price of 5$/$GJ_{BM}$.

the systematic framework developed in this thesis proves to be beneficial. The framework has the potential to be applied for studying all kinds of energy conversion systems. By expanding the superstructure with additional options, the energy market competitiveness can be accurately simulated with the aim of supporting decision-making. It turns out that process integration is a key point on which future developments have to focus.

Compared to natural gas fuelled power plants, CO_2 capture in coal fired power plants results in slightly lower cost penalty due to the larger CO_2 concentration in the flue gas. However, the energy penalty for CO_2 capture and compression leads to an energy efficiency drop to 30% for the electricity generation. Looking at the thermodynamic performance, CO_2 capture in biomass based plants can consequently compete with coal fired power plants. But coal fired power plants keep a big advantage with regard to the economic performance due to the low coal price. The specific CO_2 emissions of coal fired power plants being more than twice as high as for natural power plants, 227kg_{CO2}/GJ_e compared to 103kg_{CO2}/GJ_e, the introduction of a carbon tax will greatly penalise conventional coal fired power plants without CO_2 capture. Consequently, the introduction of a carbon tax will favour CCS and renewable biomass based processes.

In the way towards a renewable future, CO_2 capture and storage applied to H_2 and power generation plants fuelled with fossil or renewable resources, appears to be a competitive transitional solution for mitigating climate change. To reliably establish the technology on a large scale, R&D efforts should continue to address the technology availability issues and focus on the reduction of the energy and cost penalty of CCS.

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