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Thermo-environomic optimisation strategy for fuel decarbonisation process design and analysis

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ABSTRACT

To meet the CO_2 reduction targets and ensure sustainable energy supply, the development and deployment of cost-competitive innovative low-carbon energy technologies is essential. To design and evaluate the competitiveness of such complex integrated energy conversion systems, a systematic thermo-environomic optimisation strategy for the consistent modelling, comparison and optimisation of fuel decarbonisation process options is developed. The environmental benefit and the energetic and economic costs are assessed for several carbon capture process options. The 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 importance of process integration in the synthesis of efficient decarbonisation processes is revealed. It appears that different process options are in competition when a carbon tax is introduced. The choice of the optimal configuration is defined by the priorities given to the different thermo-environomic criteria.

1. Introduction

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).

Post-combustion CO_2 capture consists in the end-of-pipe separation of the CO_2 from the flue gas of fuel combustion. In oxy-fuel combustion pure oxygen is used for the combustion yielding a flue gas containing mainly CO_2 and water which is removed by condensation. In pre-combustion CO_2 capture the CO_2 is separated after the gasification and reforming of fuel and the remaining H_2 is used in a gas turbine to generate electricity.

Potential technologies for separating the CO_2 from the other gases are chemical absorption, physical ab- and adsorption and membrane processes. A detailed review of the different technologies is reported in Olajire (2010). In predictions for post 2020 scenarios from the European Union European Commission (2011) and the International Energy Agency Finkenrath (2011), 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 on the power cycle, the resources, the capture technology and the economic scenario ZEP (2012). The current status of the development of CO_2 capture technologies is reviewed in Figueroa et al. (2008). 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. The penalty of CO_2 capture in terms of efficiency and costs has been evaluated by the European Technology Platform ZEP (2011), the International Panel on Climate Change Metz et al. (2005) and the International Energy Agency Finkenrath (2011). By applying process modelling and simulations, different process configurations for producing H_2 Rosen and Scott (1998) and/or electricity Davison et al. (2010) have been evaluated considering natural gas Kvamsdal et al. (2007), coal and/or biomass resources Cormos et al. (2011), Berstad et al. (2011). These studies mainly focus on the thermodynamic performance without including detailed heat and power integration. The advantages of process integration of CO_2 capture options are investigated by Liew et al. (2014). Economic aspects of CO_2 capture are considered in Klemes et al. (2007) for coal power plants and in Bartels et al. (2010)

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ATR	autothermal reforming
BM	biomass
CAP	chilled ammonia process
CC	carbon capture
CCS	carbon capture and storage
FU	functional unit
FICFB	fast internally circulating fluidised bed
GWP	global warming potential
IPCC	international panel on climate change
LCA	life cycle assessment
LCIA	life cycle impact assessment
MEA	monoethanolamine
MILP	mixed integer linear programming
MINLP	mixed integer non-linear programming
NG	natural gas
NGCC	natural gas combined cycle
PSA	pressure swing adsorption
RME	rape methyl ester
SMR	steam methane reforming
TEA	triethanolamine

Greek letters

Δh°	lower heating value, kJ/kg
ϵ	energy efficiency, %

Roman letters

COE	electricity production cost, $/GJ$_e$
$\dot{E}$	mechanical/electrical power, kW$_e$
$\dot{m}$	mass flowrate, kg/s
$\dot{n}$	molar flowrate, kmol/s
$\dot{Q}$	heat, kW

Superscripts

+	material/energy stream entering the system
−	material/energy stream leaving the system

for plants fed with fossil or renewable resources. Environmental aspects are taken into account in Viebahn et al. (2007) and a detailed life cycle assessment of CCS in power and hydrogen plants is performed in Volkart et al. (2013), respectively in Dufour et al. (2012). However, 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 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 and a decision support approach is proposed.

2. Thermo-environomic optimisation methodology

The process design methodology combines process units and process integration models. Process modelling is realised using well established flowsheeting tools that model the process unit operations and the flows in the process superstructure. The results of the process models define the power and heat transfer requirement of the process units in the process superstructure. The process integration model is used to model the heat and mass integration of the process units to create a flowsheet from the process superstructure. The process integration model closes the overall energy balance of the system and includes the possible combined heat and power production in the system. At the end of this step the process flowsheet is completely defined and the size of the units is calculated. It is then possible to calculate the operating and capital cost of the system and to calculate the environmental performances adopting a Life Cycle Analysis (LCA) approach. The remaining degrees of freedom corresponding to operating conditions and/or selections in the superstructure are then solved using a multi-objective optimisation framework. The followed method is presented in detail in Gassner and Maréchal (2009) and the extension with the LCA in Gerber et al. (2011). The main features of the methodology are summarised in Fig. 1 and the main steps are specified hereafter.

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 MathWorks Inc (2012) based platform, 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 Tock and Maréchal (2012). 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. The trade-off between the competing objectives, like investment, emissions or energy efficiency, is assessed by multi-objective optimisation simultaneously optimising several objectives with regard to the decision variables (i.e. technology selection and operating conditions). The optimisation including discrete and continuous variables, as well as linear and non-linear relationships is a Mixed Integer Non-Linear Programming (MINLP) problem, which is solved applying a decomposition approach following a master and a slave scheme. The master optimisation realises the multi-objective optimisation search to generate the Pareto optimal sets considering the maximum energy efficiency, the minimum cost and the minimum environmental impact respectively. The decision variables of the master problem concern the operating conditions (i.e. temperature, pressure, ...) of the process units in the process structure. An evolutionary algorithm Molyneaux et al. (2010) implemented in Matlab is applied to solve the Master optimisation problem and generate a set of optimal solutions (i.e. Pareto frontier) and define the values of decision variables for the most promising configurations. The slave optimisation problem is the energy integration problem which minimises the operating cost under the heat and power cascade constraints as detailed in Section 2.2. The decision variables of the master problem are selected is such a way that the energy integration can be solved as a mixed integer linear