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Interactive Multi-objective Optimisation of Configurations for an Oxyfuel Power Plant Process for CO₂ Capture

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In this work we present a multi-objective approach to optimising configurations of an oxyfuel power plant process. The approach solves an optimisation model based on simulation results using an interactive multi-objective optimisation method, NIMBUS, which is implemented in GAMS. The optimisation model of the oxyfuel power plant process is based on simulation models of six different configurations. The simulation model is used to generate regression models for each objective, by varying the free variables that are being studied. This is done to reduce the complexity of the optimisation model. The direct results from this study suggest that it is possible to design a coal-fired power plant using an oxyfuel process, with thermal efficiency, amount of liquefied carbon dioxide and heat exchanger areas close to the ideal values. Another important result from this study is that the integration of NIMBUS and GAMS, called GAMS-NIMBUS tool, is a powerful tool to study complex processes.

1. Introduction

In this paper the interactive NIMBUS method (Miettinen and Mäkelä 2006) integrated in GAMS (2007) is used to solve a multi-objective optimisation problem for choosing the best configuration of an oxyfuel power plant for carbon dioxide capture. To be more specific, GAMS–NIMBUS tool is applied. An earlier version of it is presented in Laukkanen et al. (2010), where NIMBUS was used to solve a heat exchanger network optimisation problem. This paper is organised as follows: In the following sections the oxyfuel process and NIMBUS are described. In Section 2 the optimisation model is introduced. The results are presented in Section 3 and finally the model and results are discussed in Section 4.

1.1 Oxyfuel process

The oxyfuel power plant process is one of the routes to carbon capture and sequestration. In the oxyfuel power plant process the combustion takes place in a carbon dioxide rich environment. This is achieved by feeding (mainly) oxygen together with the fuel and recycling the carbon dioxide rich flue gas in order to control the temperature. The advantage of the oxyfuel power plant process is that the carbon dioxide is relatively easy to separate from the flue gas, as this consists mainly of water and carbon dioxide. This is at the cost of a more complicated process with lower thermal efficiency compared with a traditional power plant process. A schematic overview of an oxyfuel process is shown in Figure 1.

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Figure 1: Schematic overview of an oxyfuel process, divided into four main process parts: air separation unit, boiler, power generation and CO_2 separation unit.

The oxyfuel process is considered a viable option for so-called *clean coal* processes, and a considerable amount of research has been done in analysing both green field and retrofit conversion of coal-fired oxyfuel power plant processes, see for instance the work by Buhre et al. (2005) and Tigges et al. (2009).

Since oxyfuel combustion processes are still in the development phase, simulation and optimisation tools are needed to analyze and improve the processes. Multi-objective optimisation is a viable tool for finding and analysing efficient oxyfuel processes, because the different and conflicting design objectives can be analyzed simultaneously without the need to force these objectives into a commensurable (typically monetary) measure. To the knowledge of the authors, multi-objective optimisation, at least as a mathematical tool, has not earlier been applied in analyzing and improving oxyfuel processes.

1.2 NIMBUS - an interactive multi-objective optimisation method

NIMBUS is an interactive multi-objective optimisation method. See for instance the articles by Miettinen and Mäkelä (2006, 1999) or the book by Miettinen (1999) for a detailed description of the method. In multi-objective optimisation we have a set of optimal solutions, so-called Pareto optimal solutions with different trade-offs where the value of one objective function can be improved only by allowing impairment in some of the others. Typically, preferences of a human decision maker (DM) are used to identify the most preferred solution. The steps of the method used in this paper are the following:

- 1. Estimation of the nadir, z^{nad}, and ideal, z*, objective vectors, which provide upper and lower bounds of the objective function values in the Pareto optimal solution set.
- 2. Initialisation stage: Calculation of the first Pareto optimal solution by solving the scalarised problem (1).
- 3. The DM expresses preferences of how the current Pareto optimal solution should be improved by classifying the objective functions into up to five classes (to be described next).
- 4. Optimisation (solving problem (2) in Section 3).
- 5. The new Pareto optimal solution is presented to the DM. If the DM is satisfied with the solution, the process is complete. Otherwise the process returns to Step 3.

The problem in Step 2 that must be solved to find the first Pareto optimal solution is given as

$$\begin{split} & \text{min} \alpha + \rho \sum\limits_{i=1}^{S} \frac{f_i(x, y)}{z_i^{nad} - z_i^{**}} \\ & \text{s.t.:} \quad \alpha \geq \frac{f_i(x) - \frac{z_i^{nad} + z_i^{**}}{2}}{z_i^{nad} - z_i^{**}} \,, \quad \text{for all functions} \\ & x \in S, \end{split}$$

(1)

where $z_i = z_i + \varepsilon$ for ε is a small positive scalar, augmentation scalar, augmentation coefficient $\rho > 0$ is a relatively small scalar (e.g. 0.001) and S is the feasible region for the problem. The formula is presented for the case where all objective functions are to be minimized. In Step 3 the DM must classify the objective functions into the following five classes at the current solution:

- I[<] whose values should be improved as much as possible,
- I^{s} whose values should be improved to a desired aspiration level Z_{i} , •
- I^{\geq} whose values can get worse to a specified bound ε_{i} ,
- I⁼ whose values are acceptable and •
- I^{<>} whose values can change freely.

As the solutions presented to the DM are Pareto optimal, the DM must classify the objective functions so that at least one of the objective functions is allowed to get worse in order to obtain a new solution.

2. Formulation of the optimisation problem

In this study, an optimisation model based on simulation models of an oxyfuel power plant process with six possible configurations is formulated. The objectives functions are the thermal efficiency to be maximised, the mass fraction of liquefied carbon dioxide to be maximised and the area of all heat exchangers to be minimised, as these factors have a direct effect on the economic feasibility of the process. All the configurations have a cryogenic Air Separation Unit (ASU), a pulverized coal boiler, a steam turbine with feed water preheaters and a CO₂ separation process based on pressurizing the flue gas and liquefying the CO2. The simulation model is described in more detail in Laukkanen et al. (2008). The free variables in the optimisation model are the flow of flue gas, the pressure in the carbon dioxide condenser and the choice of any of the six configurations. With a fixed oxygen flow from the ASU, decreasing the flue gas flow i.e. decreasing the flow of recirculated flue gas increases the flue gas temperatures in the furnace. If this is technically possible (the materials in the furnace can cope with this) the power production in design mode increases. This does not happen linearly because the oxygen concentration of the flue gas is fixed, meaning that also the fuel flow changes. In this way also the flue gas flow to CO₂ Separation Process changes. The pressure of CO₂ in the final condenser affects the process, so that with increasing pressure more compression work is needed in the compressors of the CO₂ Separation Process and the net efficiency of the plant decreases.

The following process configurations are included in this study:

- 1. Conf. 1 wet flue gas circulation. Flue gas recirculation happens before water condensation. The flue gas has high water content, but a high temperature (~190 °C).
- 2. Conf. 2 dry flue gas circulation. Flue gas recirculation happens after water condensation, when the flue gas is dry, but has a relatively low temperature (~60 °C).
- Conf. 3 nitrogen in ASU molecular sieves heated by flue gas. The nitrogen needed in the 3. molecular sieves is heated by the flue gas instead of electric heaters. Flue gas circulation is wet.

- **4.** Conf. 4 low pressure feed water heating with flue gas condensing. Part of the low pressure feed water heating is done by flue gas condensation heat instead of steam. Flue gas circulation is dry.
- 5. Conf. 5 ASU intercooler heat used to preheat feed water. The ASU has only one compressor stage, and the hot air after the compressor stage is cooled by preheating the feed water replacing steam. Flue gas circulation is dry.
- **6.** Conf. 6 Low pressure feed water preheating with heat from the CO₂ separation process. Feed water preheaters are partly replaced with heat received from cooling flue gas after the first stage compressor in the carbon dioxide separation process.

The configurations are discussed in more detail in the work by Laukkanen et al. (2008).

In order to reduce the size and complexity of the optimisation model, instead of implementing the full system of equations needed to describe the process, the process is simulated and regression models are built based on the results from the simulations. The same method has been used and is described in detail in Tveit et al. (2008) and (2009). The development of the regression models is presented in the following section.

2.1 Regression models for the thermal efficiency, the mass fraction of liquified carbon dioxide and the heat exchanger area

As mentioned, the behaviour of the processes is modelled using regression models based on simulations of the process configurations to reduce the size of the optimisation problem. The different configurations have been modelled and simulated in the power plant simulation software Prosim by Endat Oy. The free variables in this study are the flue gas mass flow, pressure in the carbon dioxide compressor and which configurations have been simulated by changing the flue gas mass flow and the pressure in the carbon dioxide compressor. The regression models have been made by fitting the data to the models using the linear least square method. The coefficients for the regression models are shown in Table 1. These models are used in the implementation of the optimisation model.

2.2 Multiobjective optimisation model

The optimisation model generated by the NIMBUS method in Step 4 (for objectives to be minimised) is:

$$\min \alpha + \rho \sum_{i=1}^{3} \frac{f_{\cdot}(\mathbf{x}, \mathbf{y})}{\sum_{i=1}^{nad} - z_{i}^{**}}$$

$$st.: \alpha \geq \frac{f_{\cdot}(\mathbf{x}, \mathbf{y}) - z_{i}^{*}}{z_{i}^{nad} - z_{i}^{**}}, \forall i\{I^{\leq}\}$$

$$\alpha \geq \frac{f_{\cdot}(\mathbf{x}, \mathbf{y}) - \hat{z}_{i}}{z_{i}^{nad} - z_{i}^{**}}, \forall i\{I^{\leq}\}$$

$$f_{\cdot}(\mathbf{x}, \mathbf{y}) \leq f_{\cdot}^{j^{*}}, \forall i\{I^{\leq}, I^{\leq}\}$$

$$f_{\cdot}(\mathbf{x}, \mathbf{y}) \leq \varepsilon_{l}, \forall i\{I^{\geq}\}$$

$$f_{\cdot}(\mathbf{x}, \mathbf{y}) = \eta_{th},$$

$$f_{\cdot}(\mathbf{x}, \mathbf{y}) = x_{CO2, liq},$$

$$f_{\cdot}(\mathbf{x}, \mathbf{y}) = area_{hex},$$

$$x \in S,$$

(2)

where the variables $x \in R^2$ and $y \in Y^6$, corresponding to the free variables *i.e.* $x = [m_{fg}, p_{liq}]$ and the configurations $y = [y_1, y_2, ..., y_6]$. The feasible set *S* is made of the equations connecting the thermal efficiency, the mass fraction of the liquefied carbon dioxide and the heat exchanger areas to the free

variables and the upper and lower bounds of the variables. The feasible set also has equations that define that only one case is active at each time. The final model is implemented and solved in GAMS.

Table 1: Coefficients for the regression models of the thermal efficiency $(\eta_{th} = \beta_0 + \beta_1 \cdot m_{fg} + \beta_2 \cdot p_{liq})$, the mass fraction of liquefied CO₂ $(x_{CO_2,liq} = \gamma_0 + \gamma_1 \cdot m_{fg} + \gamma_2 \cdot p_{liq})$ and heat exchanger areas (area_{hex} = $\alpha_0 + \alpha_1 \cdot m_{fq} + \alpha_2 \cdot p_{liq})$.

	β ₀	β ₁	β2	γο	Y 1	γ 2	α ₀	α ₁	α ₂
Case 1	3.664·10 ⁻¹	- 3.792·10 ⁻⁵	- 1.132·10 ⁻³	3.845.10-1	- 4.845·10 ⁻⁵	4.288·10 ⁻²	- 6.923·10 ⁺⁷	7.037·10 ⁺⁵	9.843·10 ⁺³
Case 2	$3.122 \cdot 10^{-1}$	- 2.004·10 ⁻⁵	$2.395 \cdot 10^{-3}$	3.291.10-1	$1.112 \cdot 10^{-4}$	4.165.10-2	$4.601 \cdot 10^{+6}$	$1.228 \cdot 10^{+5}$	- 4.382·10 ⁺⁴
Case 3	3.680.10-1	- 3.668·10 ⁻⁵	- 9 .776·10 ⁻⁴	4.306.10-1	- 5.927.10-6	3.933·10 ⁻²	- 6.921·10 ⁺⁷	$7.057 \cdot 10^{+5}$	- 1.562·10 ⁺⁵
Case 4	3.645.10-1	- 2.108·10 ⁻⁵	- 1.079·10 ⁻³	3.434.10-1	$1.203 \cdot 10^{-4}$	$4.049 \cdot 10^{-2}$	$-2.452 \cdot 10^{+6}$	$1.241 \cdot 10^{+5}$	- 1.795·10 ⁺³
Case 5	$3.550 \cdot 10^{-1}$	- 4.040·10 ⁻⁵	- 1.105·10 ⁻³	3.106.10-1	$1.584 \cdot 10^{-4}$	$4.209 \cdot 10^{-2}$	$9.562 \cdot 10^{+6}$	$1.146 \cdot 10^{+5}$	- 6.516·10 ⁺⁵
Case 6	3.535.10-1	- 3.895·10 ⁻⁵	- 6.796·10 ⁻⁴	5.501.10-1	- 1.539.10-4	3.196.10-2	8.629.10+6	$1.085 \cdot 10^{+5}$	- 2.567·10 ⁺⁵

3. Results

The results of the different iterations with NIMBUS are show in Table 2.

Iteration k	Issue	Net efficiency [-]	CO ₂ recovery [%]	Area [Mm ²]
		(max)	(max)	(min)
1(Init.)	Ideal	0.344	0.92	64.77
	Nadir	0.316	0.73	75.09
	Solution	0.34	0.89	65.78
2	Classes	l≥	l<	l≥
	Initial Sol.	0.34	0.89	65.78
	Asp.lev./bound	0.33		70.00
	Opt. values	0.34	0.9	70.00
3	Classes	l≥	l<>	ľ
	Initial Sol.	0.34	0.9	70.00
	Asp.lev./bound	0.32	-	
	Opt. values	0.32	0.88	65.06
4	Classes	l⇔	l<	l [⇔]
	Initial Sol.	0.32	0.88	65.06
	Asp.lev./bound			
	Opt. values	0.32	0.92	75.09

Table 2: Results of iterations of the oxyfuel process with NIMBUS

After the fourth iteration the DM was satisfied with the solutions. As can be seen from the results the values of all objectives are reasonably close to their ideal values. Also the model solves robustly. This is partly due to the NIMBUS-method together with the efficient algorithms available in GAMS, partly due to the simulation-based simplification approach used to develop the optimisation model.

4. Discussion and conclusions

The direct results from this study suggest that it is possible to design a coal-fired power plant using an oxyfuel process with all objectives: thermal efficiency, amount of liquefied carbon dioxide and heat exchanger areas close to their ideal values. The ideal values are related to the choice of configurations made in this study. A further study, which was beyond the scope of this work, could add different costs and income to the objective values. A natural choice for costs would be other investment than heat exchanger areas and operational costs. The optimisation model could with relative ease be extended to accommodate the new objectives and the NIMBUS method is not restricted to a specific number of

objective functions. However, many more objectives can make it harder for the decision maker to manage the trade-offs between the objectives.

Another result from this study is that the integration of NIMBUS and GAMS, called GAMS-NIMBUS tool, is a powerful tool for studying complex processes. The authors are confident that a fully multi-objective approach to the conceptual design of oxyfuel processes will be a valuable aid to decision makers. The multi-objective approach gives the decision maker a better opportunity to understand the underlying trade-offs between the objectives and gain a better understanding of the processes than single-objective optimisation.

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