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Dynamic Real-Time Optimisation of a CO_2 Capture Facility

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Abstract: This work investigates economic optimisation of an energy-intensive amine regeneration process in a post-combustion CO_2 capture plant, subject to a minimum CO_2 capture ratio over 24 hours. A Dynamic Real-Time Optimisation algorithm is implemented as a single-level Nonlinear Model Predictive Control scheme by utilising the infeasible soft-constraint method to include economic objectives in an industrial tracking NMPC package. A time-varying price of electricity is exploited to enhance cost minimisation by adjusting the regeneration according to the peaks of the price curve. This flexible mode of operation is compared to a fixed mode of operation with constant amine regeneration. Simulation results indicate a cost reduction of 10.9% for a reference accumulated capture ratio of 91%. Robustness of the optimisation to abrupt changes in CO_2 feed composition and electricity price is also investigated in simulations and results are promising. The NMPC controller uses a reduced, control-oriented model of the capture plant developed from first principle conservation laws with control volumes to discretize the model equations in space.

Keywords: dynamic real-time optimisation, nonlinear model predictive control, model-based optimisation and control, CO2 management

1. INTRODUCTION

According to WMO (World Meterological Organization, 2017), 2017 was among the three warmest years on record. WMO states that the climate changes are most likely caused by the increase of human-made greenhouse gas emissions into the atmosphere, the most prominent being CO_2. A promising technology for reduction of CO_2 emissions is post-combustion carbon capture which may capture CO_2 from the exhaust gas of power plants and industrial processes. However, Smith et al. (2013) found that power plants with a CO_2 capture plant attached to the outlet had an increase in operational costs in addition to decreased efficiency. To make carbon capturing more desirable and profitable, contributing towards reduced greenhouse gas emissions and possible stalling of global warming, reduction of the operational costs is of high importance.

A post-combustion CO_2 capture facility may for instance use absorption with monoethanolamine (MEA) to remove the CO_2 component of the exhaust gas (Carbon Capture and Storage Association, 2018). In the absorption tower of the plant, a liquid MEA solution will encounter the exhaust gas and absorption occur due to a reaction between the MEA and the CO_2. In the desorption tower, the reverse process occurs where the liquid MEA is regenerated and a nearly pure stream of CO_2 is let out. Desorption is a highly energy-demanding process as the liquid must be heated sufficiently for the MEA to release the CO_2.

The objective of this work has been to minimise the cost related to the energy consumption of the MEA regeneration through 24 hours while regulating the system to a reference accumulated capture ratio. With that horizon in mind, the optimisation algorithm should be able to exploit an hourly varying price of electricity to enhance cost minimisation, imposing less regeneration during high peaks and more regeneration during low peaks. The paper is structured such that firstly, in Section 2, the model of the capture plant used for optimisation is introduced and validated regarding modelling errors and system stiffness. Secondly, Section 3 presents theory and formulation of the dynamic real-time optimisation problem and describes the industrial tracking NMPC package from *Cybernetica AS* that has been used for simulation. Simulation results are illustrated and discussed in Section 4 and lastly, conclusive remarks are made in Section 5.

2. MODEL

An existing mechanistic model of a CO_2 capture plant was made available by *Cybernetica AS* for this work. The model, referred to as the *original* model, is a slightly adjusted version of the model in Flø (2015) and is in fact based on a test facility located at Tiller in Trondheim (SINTEF, 2017). The model used for optimisation of the capture plant is a reduced version, in terms of state space complexity, of the original model, and will consequently be referred to as the *reduced* model. Similarly to the original model, the mass and energy balance equations for the reduced model was developed using first principle conservation laws. However, for three of the unit models in the plant; the absorber, desorber and heat exchanger,

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were molar amounts instead of molar flows of each substance used as state variables and the system discretized in space using the control volume method instead of the collocation method. Due to page restrictions, the details and development of the dynamical equations have not been included but may be found in Hotvedt (2018). The reduced model was validated against the original model using *Cybernetica AS*'s offline model validation tool Modelfit and an analysis of the system stiffness and computational effort was performed. The validation has been performed disregarding modelling errors from the true facility at Tiller as the original model yielded satisfactory responses when *Cybernetica AS* tested its responses against instrumental measurements provided by SINTEF.

The model validation in Modelfit utilised a pre-generated data set of inputs from SINTEF to simulate the responses of the two models. The data set consisted of K = 4656 samples, representing feasible combinations of inputs for more than 3 days. Two variables have been compared considering modelling errors between the original and the reduced model, the capture ratio (CR) in the absorber column,

$$CR = 100 \cdot \frac{F_{g,abs,CO_2,in} - F_{g,abs,CO_2,out}}{F_{g,abs,CO_2,in}} \tag{1}$$

and the mass flow of CO_2 from the condenser $F_{g,cond,CO_2}$. Here F_{g,abs,CO_2} is the flow of gas of CO_2 in or out of the absorber. The responses were analysed using maximum and average absolute deviation

$$\begin{aligned} \max|\tilde{D}| &= \max_k \left(|\phi_{org,k} - \phi_{red,k}|\right) \\ avg|\tilde{D}| &= \frac{\sum_{k=0}^{K}\left(|\phi_{org,k} - \phi_{red,k}|\right)}{K} \end{aligned} \tag{2}$$

Here ϕ is a generic variable and subscripts org and red represent the variable in the original and reduced model. The result may be seen in Table 1 and an illustration of the model responses are presented in Fig. 1.

Table 1. Maximum and average absolute deviation of the capture ratio and the mass flow of CO_2 from the condenser.

Case	Variable	max $\mid \tilde{D} \mid$	avg $\mid \tilde{D} \mid$
Without parameter adjustment	CR [%]	27.68	11.21
	$F_{g,CO_2,cond}$ $[\frac{kg}{h}]$	11.10	3.18
With parameter adjustment	CR [%]	25.25	2.32
	$F_{g,cond,CO_2}$ $[\frac{kg}{h}]$	12.63	0.85
With bias updating	CR [%]	29.54	1.20
	$F_{g,cond,CO_2}$ $[\frac{kg}{h}]$	11.68	0.55

As may be seen from the results, a bias between the original and reduced model is present, most likely due to the reduced model having fewer states and therefore likely to loose accuracy. What may also be noticed from the bottom figure in Fig. 1, is that the variable $F_{g,cond,CO_2}$ in both the original and reduced model deviate from the instrumental measurement provided by SINTEF, illustrated as the dashed line. This deviation is due to the simplifications being made modelling the process. Manual parameter adjustments of the reduced model decreased the average absolute deviation from the original model, however, complete removal was not straightforward. Consequently, a simple estimator based on bias updating was introduced. Bias updating compares instrumental measurements to the modelled variable on each time step, scales the deviation with an appropriate constant parameter determined in advanced, and introduces the scaled error back into the model. In this work, the measurements of the $F_{g,cond,CO_2}$ was utilised to update not only the $F_{g,cond,CO_2}$, but also the capture ratio as there is a close correspondence between the two variables. As may bee seen from the bottom row in Table 1, the average absolute deviation of the $F_{g,cond,CO_2}$ and the CR decreased further with the use of bias updating. A disadvantage with bias updating is that the variables to be updated, in addition to the update parameter, must be determined in advance of simulation. A Kalman Filter could take advantage of the measurements to automatically find which states or parameters to update for a better model response. Development of an extended Kalman Filter would be a natural next step, but not included in this work. Notice however, *Cybernetica AS* found that combining the original model with an EKF was too computationally demanding for use in online estimation and optimisation.

The stiffness of the two models was investigated through an eigenvalue analysis. Stiffness is a property that often occurs when both fast and slow dynamics are present in the model. This may influence the solving time of the system as the step size in integration routines must be set small to account for the fastest dynamics. Stiffness may be analysed using the Stiffness Ratio (Moody, 2007)

$$SR = \frac{\max_i |\Re(\lambda_i)|}{\min_i |\Re(\lambda_i)|} \tag{3}$$

where λ_i for $i \in R^m$ are the eigenvalues of the Jacobian matrix of the system, which for a nonlinear system may be approximated using finite differences. An $SR >> 1$ characterise a stiff system. The eigenvalue analysis was performed in both dynamic and steady state, however, the results show an $SR >> 1$ for both models. On the other hand, the use of the control volume method resulted in a halving of the state space dimension of the reduced compared to the original model, see Table 2, which further led to a simulation time reduction of approximately 73%. Consequently, the reduced model may be better suited for use in online estimation.

Table 2. Comparison of state space dimension and simulation time from Modelfit for the original and reduced model

Model	State space dimension	Simulation time (s)
Original	448	≈ 26
Reduced	223	≈ 7

3. DYNAMIC REAL-TIME OPTIMISATION

The optimisation problem for the CO_2 capture facility has been formulated as a Nonlinear Model Predictive Control (NMPC), where the industrial NMPC tool CENIT from *Cybernetica AS* has been employed to solve the optimisation. CENIT is designed to handle highly nonlinear models using nonlinear mechanistic models in addition to online model adaption for adjustments of deviations away from the true process (Cybernetica AS, 2018). Both economic and regulatory objectives were included in the

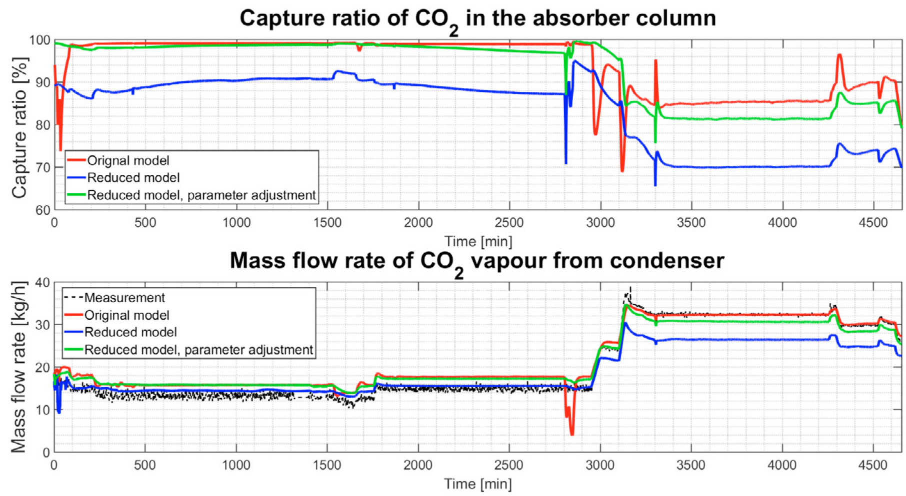

Fig. 1. Result of capture ratio in the absorber column and mass flow of CO_2 from the condenser comparing the original and the reduced model

optimisation, the economic being minimisation of the cost related to the energy consumption in the reboiler and the regulatory being reference tracking for the accumulated capture ratio. Common in literature (Arce et al., 2012; Manaf et al., 2017), is the use of a two-level control hierarchy where both economic and regulatory objectives are considered. The upper level providing economic optimal set-points to the lower level which controls regulatory performance. However, several authors (Kadam et al., 2003; Engell, 2007; Maree and Imsland, 2011) points out that a disadvantage with the two-level hierarchy is an often sub-optimal economic performance and suggests merging of the objectives into one level. Such a control structure is sometimes referred to as Dynamic Real-Time Optimisation (DRTO) or Economic Model Predictive Control (EMPC). In Willersrud et al. (2013), two methods for implementation of the DRTO was investigated, the unreachable setpoints method (Rawlings et al., 2008) and the infeasible soft-constraint method. However, Willersrud et al. (2013) points out that the unreachable setpoint in the first method may affect the optimal solution because of its appearance in the KKT conditions. Consequently, the infeasible soft-constraints method has been implemented for the CO_2 capture facility. During development and experimentation with the DRTO, *Cybernetica AS*'s tool RealSim has been utilised to simulate the true process using the original model. Consequently, RealSim has been examined to see how well the optimal outputs from CENIT, calculated using the reduced model, affects the carbon capture plant, simulated with the original model, in addition to making measurements, simulated with the original model, available for online model adaption of the reduced model through bias updating.

3.1 Single-level NMPC

The infeasible soft-constraint method has been illustrated in Fig. 2 for both maximisation and minimisation problems. The method introduces out-of-bounds constraints on the economic objectives and includes slack variables, ε, in the objective function to represent the deviation away from the constraints. The optimisation problem will hence be

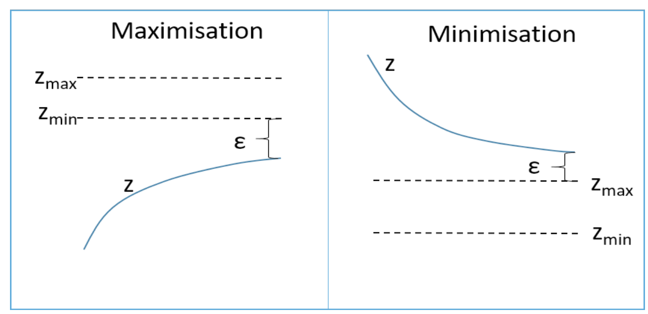

Fig. 2. Illustration of the infeasible soft-constraint method for single-level MPC

feasible but minimise the deviations as much as possible. The same derivation as in Willersrud et al. (2013) but for minimisation instead of maximisation, has been utilised to write the objective function in an NMPC scheme with a linear optimising term for the economic objectives as follows

$$\begin{aligned}\min_{\phi \in R^n} f(\phi) = \sum_{i=0}^{N-1} &(\mathbf{z}_{reg,i+1} - \mathbf{z}_{reg}^{ref}) Q_{reg} (\mathbf{z}_{reg,i+1} - \mathbf{z}_{reg}^{ref}) \\ &+ \Delta \mathbf{u}_i^T R_\Delta \Delta \mathbf{u}_i \\ &+ \rho_{reg}^T \varepsilon_{reg,i+1} + \rho_{opt}^T \mathbf{z}_{opt,i+1}\end{aligned} \tag{4}$$

with N as the prediction horizon. The objectives were divided in two, regulatory $\mathbf{z}_{reg}$ and economic $\mathbf{z}_{opt}$ and the matrix for the quadratic term set to

$$Q = \begin{bmatrix} Q_{reg} & 0 \\ 0 & 0 \end{bmatrix} \tag{5}$$

Further, it has been used that minimisation of ε_{opt} yields the same result as minimisation of $\mathbf{z}_{opt}$. This may be stated if the upper and lower constraints on the economic objectives are chosen such that $\mathbf{z}_{opt,min} \leq \mathbf{z}_{opt,max} \leq \mathbf{z}_{opt}$ and $\varepsilon_{opt} = \mathbf{z}_{opt} - \mathbf{z}_{opt,max} \geq 0$. If ρ_{reg} and ρ_{opt} are large, this will in effect become an exact penalty function for the constraints (Nocedal and Wright, 2000). Practical considerations such as desired closed-loop behaviour and numerical conditioning often dictates lower values in practice.

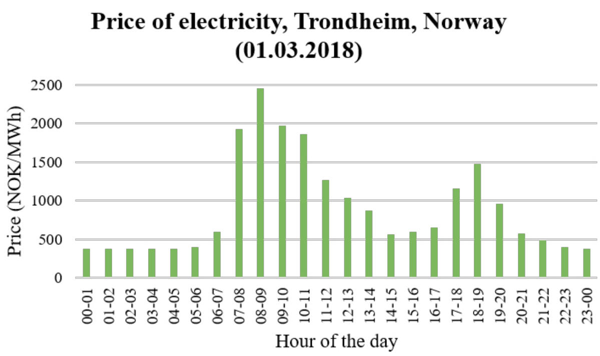

Fig. 3. Illustration of the time-varying price of electricity in Trondheim, Norway collected from Nord Pool (2018)

3.2 Formulation of optimisation problem

Two different objective functions, resulting in two different modes of operation, were considered and compared to each other. Firstly, a flexible mode of operation in which the main regulatory objective, the accumulated capture ratio

$$CR_{acc} = 100 \cdot \frac{\int_0^k (F_{g,abs,CO_2,in} - F_{g,abs,CO_2,out})dt}{\int_0^k F_{g,abs,CO_2,in}dt} \quad (6)$$

was allowed to vary during the simulation horizon as long as its reference CR_{acc}^{ref} was obtained at $N = 24$ hours. Secondly, a fixed mode of operation where the CR_{acc} was forced to its reference value throughout the horizon. In both modes of operation was the economic objective of the problem to minimise the cost

$$Cost = \int_0^k \psi \cdot RDdt \quad (7)$$

related to the energy consumption of the amine regeneration process in the reboiler, reboiler duty (RD). The price of electricity, $\psi(t)$, is time-varying and illustrated in Fig. 3 with data collected from Nord Pool (2018). Thus, in the flexible mode of operation should the solution of the optimisation indicate exploitation of $\psi(t)$ by varying the CR_{acc}, and hence the amine regeneration, according to the peaks of the price curve. In this work ψ is deterministic and pre-determined. A natural next step would be to develop an outside algorithm for electricity price predictions using for instance weather forecasts and data from similar situations.

The instantaneous capture ratio (CR) in (1) were in both modes regulated within the bounds (min, max) = (75, 96)%. This was to avoid a complete shutdown of the capture facility for low CR and to avoid large model uncertainties for large CR. Thus, three controlled variables (CV), $\mathbf{z}$, were utilised for optimisation. The CR_{acc} and CR as the regulatory objectives $\mathbf{z}_{reg}$, and the cost as the economic objective z_{opt}. Controlled variable evaluation points were utilised to decrease the number of constraints of the optimisation problem (Strand and Sagli, 2004). In the flexible mode of operation, one evaluation point at 24 hours was enough for the CR_{acc} to reach the objectives. For the fixed mode of operation, 6 evaluation points evenly spread out were needed to force the CR_{acc} to its reference throughout the horizon. In both modes of operation were 6 evaluation points necessary to keep

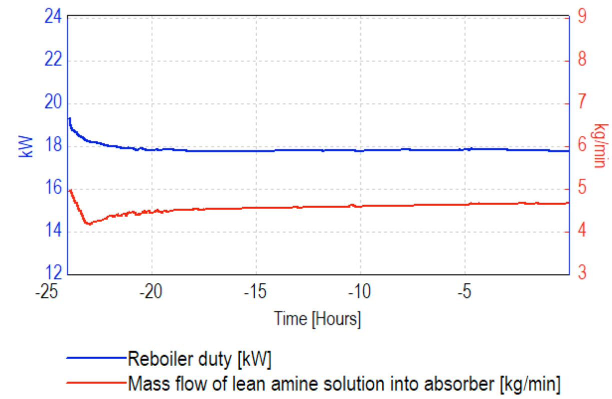

Fig. 4. Result of the Manipulated Variables for the fixed case with $CR_{acc}^{ref} = 91\%$

the CR within its bounds. Notice, the prediction horizon in a standard NMPC is receding and thus to ensure that optimum is reached after exactly 24 hours, the variables must be "frozen" at $k = 24$ hours. To achieve this in practice, the integrals are not updated after this point in time when the control horizon goes beyond this point. Two manipulated variables (MV), $\mathbf{u}$, were chosen, the RD and the mass flow of lean amine into the absorber $F_{l,abs}$. Input blocking was utilised to reduce the degrees of freedom of the problem (Maciejowski, 2002). As the price of electricity changes every hour of the day, 24 input block's would be ideal, however, 12 input block's evenly spread out yielded sufficient performance.

4. RESULTS OF OPTIMISATION

A reference accumulated capture ratio of $CR_{acc}^{ref} = 91\%$ were utilised in the simulations and an optimal solution accepted if the result in CENIT was within $CR_{acc}^{ref} \pm 0.2\%$. To simplify the tuning of the controllers, online model adaption from the simulated facility in RealSim was turned off. However, the outcome in RealSim was examined to ensure that the optimal solution in CENIT was credible. The results of the MV's and CV's from CENIT for the fixed case may be seen in Fig. 4 and Fig. 5 and for the flexible case Fig. 6 and Fig. 7. The flexible case resulted in a cost reduction of 10.9% compared to the fixed case as the amine regeneration could be adjusted according to the peaks of the electricity price curve. Keep in mind that the simulations were run from a high initial point resulting in a warm start. As a consequence, the DRTO could focus on decreasing the CR_{acc} towards reference. A lower initial point may have resulted in decreased cost reductions. It was found that the simulated facility in RealSim yielded a larger end CR_{acc} than the reference value, suggesting an unnecessary use of RD. Consequently, online model adaption was turned on with the inclusion of bias updating from measurements of $F_{g,CO_2,cond}$. The result was a smaller end CR_{acc} in RealSim and thus lower cost. However, bias updating was only experimented briefly with and should be further investigated to enhance cost minimisation.

Furthermore, the robustness of the optimisation was tested in three scenarios; to an abrupt change in CO_2 feed composition, to an abrupt change in electricity price and

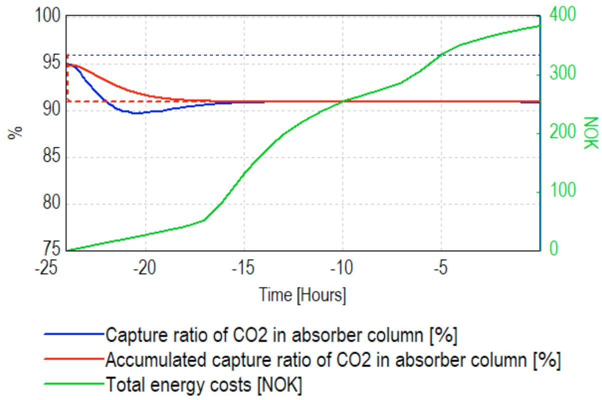

Fig. 5. Result of the Controlled Variables for the fixed case with $CR_{acc}^{ref} = 91\%$

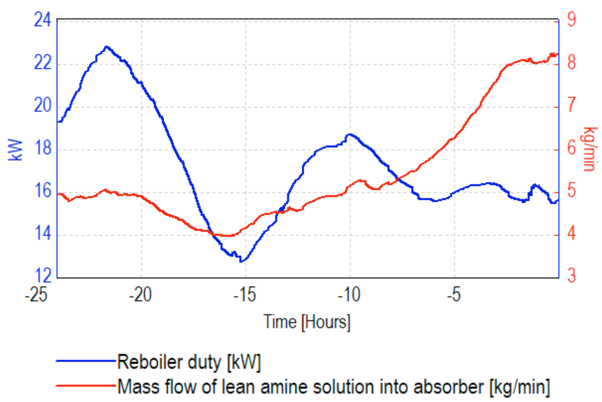

Fig. 6. Result of the Manipulated Variables for the flexible case with $CR_{acc}^{ref} = 91\%$

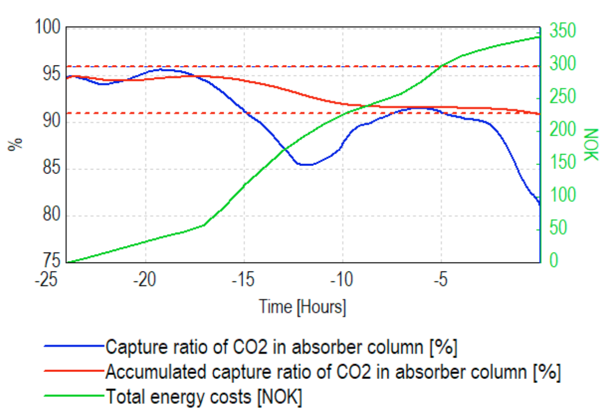

Fig. 7. Result of the Controlled Variables for the flexible case with $CR_{acc}^{ref} = 91\%$

for stricter constraints on the RD. For the abrupt changes in CO_2 feed composition was the DRTO able to re-plan the optimal solution and reach the CR_{acc}^{ref} if the change did not happen close to the end of simulation horizon. A successful simulation where the change occurred after 11.5 hours is shown in Fig. 8 and Fig. 9. For all abrupt changes in the electricity price was the DRTO able to reach CR_{acc}^{ref}. Furthermore, if the change occurred early in the simulation was the DRTO able to re-plan the optimal solution to enhance cost minimisation. An a example

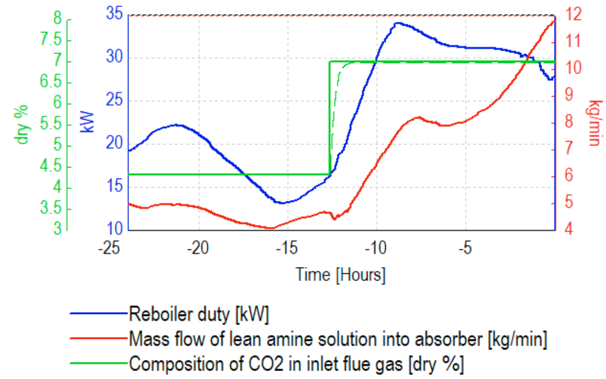

Fig. 8. Result of the Manipulated Variables for the flexible case with an abrupt change in CO_2 feed composition after 11.5 hours, $CR_{acc}^{ref} = 91\%$

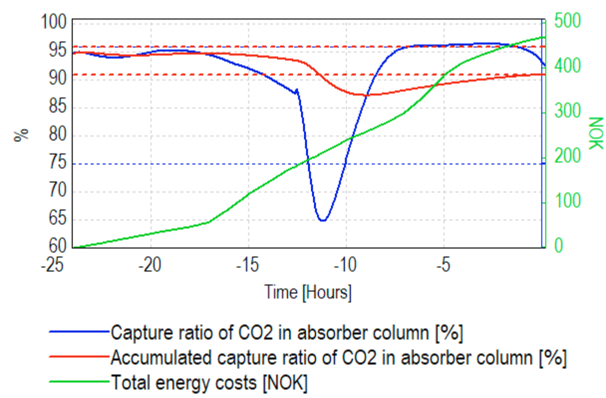

Fig. 9. Result of the Controlled Variables for the flexible case with an abrupt change in CO_2 feed composition after 11.5 hours, $CR_{acc}^{ref} = 91\%$

of this is illustrated in Fig. 10 and Fig. 11 where the change occurred after 4.5 hours. Notice, comparing the MV's to the standard flexible case in Fig. 6, that the RD is somewhat smaller during the high peaks of the electricity price and somewhat larger during the low peaks occurring after 4.5 hours. For the simulation case with stricter constraints on the RD was the DRTO able to reach the CR_{acc}^{ref}. However, the RD had to be varied less to keep it within the constraints, naturally leading to higher costs. Due to limited space is the last mentioned simulation case not illustrated but may be found in Hotvedt (2018).

5. CONCLUDING REMARKS

The reduced model developed and analysed in Section 2 induces a simulation time reduction of 73% compared to the original, and will consequently be better suited for use in online estimation and optimisation. Model deviations between the original and reduced model are present, however, results indicate that bias updating from measurements can alleviate the errors significantly. Results from Section 3 show that the use of a DRTO based on a single-level NMPC for merging economic and regulatory objectives yields satisfactory results. Two different modes of operation is investigated, a flexible mode where the amine regeneration is varied according to the peaks of a time-varying price of electricity and a fixed mode where

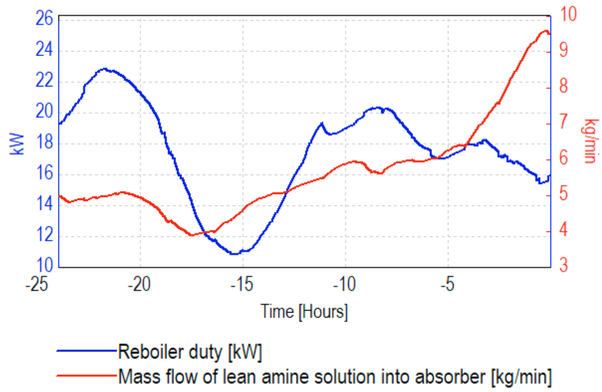

Fig. 10. Result of the Manipulated Variables for the flexible case with an abrupt increase in price of electricity after 4.5 hours, $CR^{ref}_{acc} = 91\%$

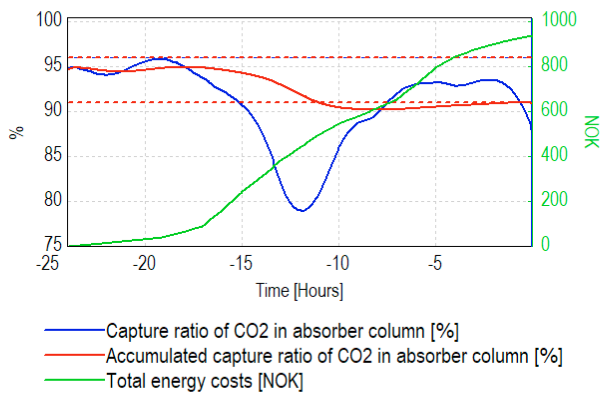

Fig. 11. Result of the Controlled Variables for the flexible case with an abrupt increase in price of electricity after 4.5 hours, $CR^{ref}_{acc} = 91\%$

the amine regeneration is held constant. Results suggest that the flexible mode of operation induces a cost reduction of 10.9% compared to the fixed mode. It is further illustrated that the DRTO is robust to abrupt changes in the electricity price and abrupt changes in the CO_2 feed composition as long as the change do not occur close to the end of prediction horizon. Further work with the model and optimisation problem should experiment with replacing bias updating with a nonlinear state estimator such as the Kalman Filter, potentially removing deviations from the true process and enhancing cost minimisation.

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