Process synthesis and controllability assessment of CO_2 capture plants in a parallel environment

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The objective of this work is to develop, implement and evaluate a parallel computational framework for the simultaneous process synthesis and controllability assessment of absorption/desorption processes for post-combustion CO_2 capture. The framework employs a stochastic optimisation algorithm which is able to handle efficiently discrete design variables, pertaining to process flowsheet structural features represented through a generic superstructure. The discrete design parameters are introduced iteratively into a deterministic optimisation algorithm which is efficient for continuous design variables and operates internally within the stochastic algorithm. Every solution obtained by the continuous algorithm is transferred into a controllability assessment stage, implemented in the form of a non-linear sensitivity analysis approach which evaluates the effect of disturbances within an optimum control scheme. This layout is realized within a synchronous, parallel realization of a Simulated Annealing algorithm, where the primal-dual interior-point optimisation algorithm, as implemented by the Interior Point Optimizer (IPOPT) software, is used for steady-state process design and the predictor-corrector homotopy-continuation algorithm, using the PITCON software, for controllability assessment. The obtained results show that the parallelisation scheme is computationally very efficient and the obtained solution is 52 % better in terms of overall performance than a corresponding, conventional sequential process design and control approach.

1. Introduction

The synthesis and design of absorption/desorption flowsheets by using optimisation procedures has received increased attention in recent years as a means of reducing the capital and operating costs associated with CO_2 capture, as reported in Papadopoulos and Seferlis (2017). The optimal process operation point cannot always be guaranteed due to several exogenous disturbances, which may cause complete shifting of the process from its nominal and already proposed optimal solution point. Typical examples of such disturbances are associated with changes in the composition and volumetric flowrate of the flue gas, ambient conditions that may affect the operating conditions of the plant and imposed changes in the operating policy of the plant itself. Therefore, the performance of the plant at off-design operating points may significantly deviate from desired economic targets for CO_2 capture. Evidently, there is a need for simultaneous consideration of process economics and controllability assessment of the plant design under these varying process conditions. However, the vast number of structural and operating options that need to be considered in view of disturbances result in prohibitive computational challenges.

Currently, there are numerous approaches reported in published literature that propose integrated process design and controllability assessment. On the work of Kyriakides et al. (2019), the authors present an integrated process design and control framework for a membrane-based hydrogen production system based on low temperature methane steam reforming using an advanced control system under multiple disturbance scenarios. Furthermore, several alternative flowsheet configurations are designed and assessed by taking into consideration the economic and controller dynamic performance criteria simultaneously. Hauger et al. (2019)

present an optimal control solution based on nonlinear model predictive control (NMPC) for post-combustion CO_2 capture processes to keep the CO_2 capture ratio at a desired level while minimising the reboiler duty. In a similar base, a NMPC control strategy is also used by Zhang et al. (2019) and compared with the traditional proportional-integral-derivative (PID) controller. Moreover, a robust controller is developed for the control of a CO_2 capture plant with due consideration of model uncertainty. A dynamic real time nonlinear optimisation framework for estimation and control is demonstrated by Thierry and Biegler (2019), along with a case study of a bubbling fluidized bed reactor for CO_2 capture. A comprehensive summary of different methods and a detailed classification regarding the integrated design and control of chemical process can be found on the work of Vega et al. (2014). The aim of all these approaches is to reduce the computational effort while considering interactions between process design and controllability features of the problem. However, quite often the employed process representations are limited to mainly operating options, whereas structural flowsheet changes are rarely considered in combination with different control structures under multiple disturbance variations. Furthermore, solutions are obtained using local optimisation algorithms. Even in such approaches, computational challenges are mainly addressed through arbitrary reduction of process design decisions, operating interactions and disturbance effects, therefore hindering the identification of improved solutions.

2. Motivating problem

The design of absorption/ desorption processes for CO_2 capture can be greatly benefited by the consideration of flowsheet modifications in order to improve the process economics (Damartzis et al., 2014). This is performed systematically through generic representations of process layouts, also known as superstructures, to avail a rich pool of design decisions and design advanced absorption/desorption process flowsheets for post-combustion CO_2 capture. The employed superstructure consists of different modules representing generic process tasks such as chemical reactions, mass separation, heat transfer, and so forth. A mathematical model is assigned to each module representing a particular task. This modular approach provides great flexibility and allows easy generation of various flowsheet configurations. In addition, the orthogonal collocation method on finite elements (OCFE) technique is employed, approximating the molar and enthalpy flows inside each module. By the use of Lagrange polynomials, the transformation of the complex equations of the underlying model in study, into continuous polynomial functions of the module's length is achieved. More details regarding the above method are reported in the work of Damartzis et al. (2014). The main advantage of OCFE is the characterisation of complex phenomena in a compact way (i.e., reduction of total number of modeling equations) in combination with low computational cost and satisfactory accuracy in model predictions. In this study, a generic superstructure is used with double section stripper and intercooled absorber (DSS-ICA), as in Damartzis et al. (2018), and an aqueous solution of monoethanolamine (MEA) 30 % wt. is chosen in order to absorb and separate CO_2 from an industrial flue gas stream.

3. Proposed approach

3.1 Approach overview

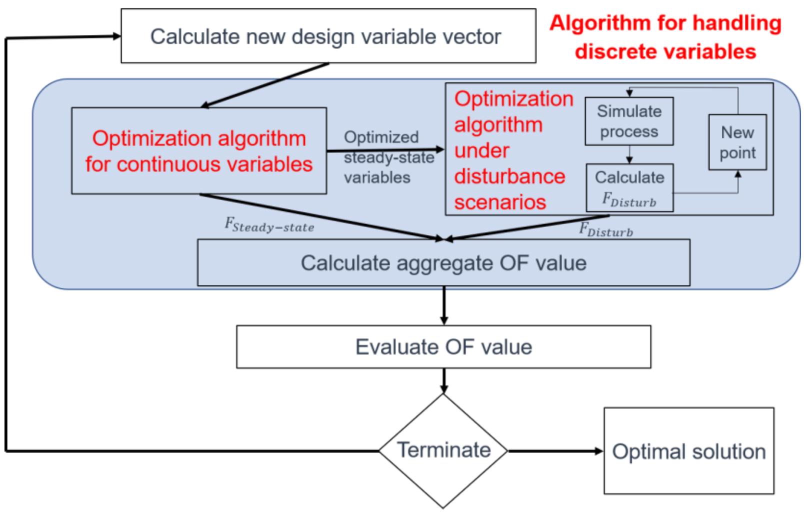

Figure 1: Generic solution procedure of the approach, invariant of the algorithms used.

In this work, the simultaneous synthesis of absorption/desorption flowsheets under the influence of disturbances using a parallel optimisation approach is proposed. Unlike previous works, a generic superstructure for the representation of process design decisions is employed, following the work of Damartzis et al. (2018), which is combined with a systematic controllability assessment framework. The latter quantifies and assesses the sensitivity of different structural and operating options in the course of process optimisation for different and multiparametric disturbance scenarios. The optimisation is performed through a parallel implementation of a stochastic search method, combined with derivative-based algorithms. Prior to elaboration of the parallelisation approach, Figure 1 illustrates the main stages of the optimisation approach, which combines a stochastic optimisation algorithm to handle discrete decision variables with a local deterministic optimisation algorithm for continuous decision variables.

The stochastic optimisation algorithm provides mechanisms to target the globally optimum domain in the context of a superstructure flowsheet representation that includes numerous discrete design decisions. The deterministic algorithm performs rigorous local searches considering continuous decision variables, within the range of the imposed discrete parameter space. Controllability assessment is addressed through a nonlinear sensitivity analysis approach, simultaneously with process design. In particular, the stochastic optimisation algorithm is used to handle discrete decision variables externally to the emulator of the physical material and process model. The latter includes different structural flowsheet configurations assigned to different/parallel computational units (e.g., cores, threads and so forth). For each set of discrete parameters, the deterministic optimisation algorithm uses continuous operating conditions as decision variables and performs optimisation based on an objective function ($F_{Steady-state}$) corresponding to each structural configuration. Subsequently, for each structural configuration, the solution obtained from the deterministic algorithm is investigated under the influence of multiple disturbances using a criterion ($F_{Disturb}$) that measures the deviation of the process variables from their target optimal values. The latter is performed within a nonlinear sensitivity analysis framework (Seferlis and Grievink, 2004) using an algorithm that computes a sequence of solution points along a one-dimensional manifold of a system of nonlinear equations.

3.2 Parallelisation scheme

To enable the investigation of a wide process design and disturbance space, the parallelisation of the time-consuming simulations of the process model for different realizations of the discrete and continuous variables as well as of the disturbances is proposed. Such simulations are implemented internally by the deterministic optimisation algorithm and by the controllability assessment approach (Figure 1) in order to obtain the optimal design and to assess its performance under multiple disturbance scenarios. Although the presented approach is generic, the parallelisation scheme is tailored to the requirements of the employed stochastic optimisation algorithm.

The proposed computational framework consists of three different algorithms, each one executing a particular task and contributing to a different detail in the overall approach. In particular, the first algorithm used is Simulated Annealing (SA) (Kirkpatrick et al. 1983), which is a stochastic optimisation technique. Its mathematical formulation is based on probability theory and Markov processes and provides venues to target the globally optimum solution or a close approximation of it. A variation of a parallel version of the aforementioned algorithm proposed by Ferreiro et al. (2013) is utilised to handle the discrete variables of the process. A starting temperature T_0, a predefined number of iterations within every temperature level (Markov chain length-LMC), a starting point $\mathrm{X}s$ (blue square in Figure 2), and bounds for the variables of the design vector X are necessary for the initialisation of the algorithm. For each Markov chain iteration of every parallel process, i.e. the green squares, as shown in Figure 2, under the current temperature level, a new randomly selected move X_{m} is applied, starting from the previously accepted move $\mathrm{X}_{\mathrm{m}}^{\mathrm{min}}$ and a set of discrete parameter values (i.e. structural variables of the process system such as the discretised lengths of the absorber/stripper column) is transmitted to every computational unit.

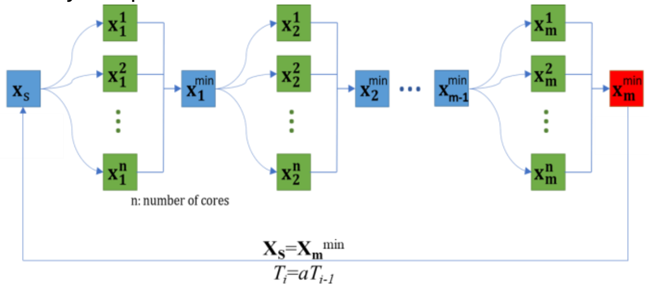

Figure 2: Synchronous parallel simulated annealing algorithm architecture.

Afterwards, for each set of discrete variables, a primal-dual interior-point optimisation algorithm for nonlinear programming (IPOPT), developed by Wächter and Biegler (2016), uses the continuous variables as decision variables and performs optimisation in the sense of minimising the objective function ($F_{Steady-state}$), which corresponds to each structural instance. Subsequently, the optimal solution obtained from the previous step (IPOPT) is investigated under the influence of multiple disturbances within a nonlinear sensitivity analysis framework using a predictor-corrector continuation method as implemented by the software PITCON, developed by Rheinboldt and Burkardt (1983). In essence, the green squares of Figure 2, execute in parallel multiple different realisations of discrete and continuous variables and disturbance scenarios. For a fixed temperature, each computational process/thread i.e. n cores, runs for all LMC and reports its value. When all threads are finished, that is for every thread the optimised continuous design variables have been calculated and the controllability assessment has been determined, the Metropolis criterion, Metropolis et al. (1953), is employed by SA in order to obtain the next valid design state x_i, that corresponds to the minimum F_{obj} of all the computational units. The latter is the sum of both $F_{Steady-state}$ and $F_{Disturb}$, hence both the steady state and off-design economic performance are evaluated. Notice that the parallelisation scheme is essentially implemented within the Markov Chain iterations. Once all iterations are completed (red square in Figure 2), the temperature is updated and the algorithm continues until the termination criteria are satisfied.

4. Implementation

4.1 Process design problem formulation

An aggregate objective function comprised of the sum of the objectives of each subproblem of the form

$$\min F_{obj} = F_{Steady-State} + F_{Disturb} \quad (1)$$

is utilised. Due to the OCFE formulation by Damartzis et al. (2014), every column is separated into finite elements. In this case, the absorber and the stripper column are both divided into three elements to make up a total of six elements. The length of each element is considered a discrete variable and all together constitute the variables handled by the stochastic algorithm. The first term, $F_{Steady-state}$, of Eq(1), is the economic cost function of the process in steady state conditions, encapsulating the capital and operating expenses while aiming to preserve the CO_2 at a desirable level. The selected objective function has the form

$$F_{Steady-State} = C_{abs} + C_{str} + C_{hex} + C_{reb} + C_{pump} + C_{wat} + C_{amine} + C_{cool} + C_{steam}. \quad (2)$$

The first two terms express the total cost of the columns used, namely the absorber and the stripper column. These two are highly dependent on the selected columns length. The third term includes the total expenses of the heat transfer units employed that is the heat exchanger, the condenser at the top of the stripper column, the cooler and the intercoolers responsible to cool the absorber. The next in the above equation C_{reb}, characterise the reboiler unit cost and the C_{pump} term express the cost of the pump equipment to keep the liquid flowing between the columns. The above-mentioned refer to the capital costs, whereas the last four terms of Eq(2) indicate the operating costs. The latter include C_{wat} and C_{amine} which are the total costs of water and amine respectively used in the process as well as the make-up amount in order to counter-balance the losses. C_{cool} stands for the expenses regarding the cooler and the intercoolers and lastly C_{steam} is the cost of steam consumed for the operation of the reboiler unit. Every design variable, other than the absorber and stripper lengths, is considered continuous and the locally optimal values which minimise the objective function of Eq(2) subject to the model constraints are sought. Among them, the ones with increased interest are the CO_2 loading of lean and rich flow stream that feed the absorber and the stripper respectively, the lean solvent flow rate, the duties of the cooler, intercoolers, condenser and reboiler. In addition, the temperature of the reboiler is of great importance along with the pressures at the bottom of the absorber and desorber. Finally, the split ratio of the rich stream that feeds the stripper at two points is to be optimised.

4.2 Controllability assessment problem formulation

Following the work of Damartzis et al. (2018), the controllability assessment framework is formulated as an optimisation problem in order to evaluate the steady-state response of the process under the various exogenous disturbances, as follows:

$$F_{Disturb} = \left(x - x_{sp}\right)^T W_x \left(x - x_{sp}\right) + \left(u - u_{sp}\right)^T W_u \left(u - u_{sp}\right) \quad (3)$$

The above equation denotes the disturbance cost function and is the second term of Eq(1), where x and u represent the controlled and the manipulated vector variables respectively, $[x_{sp}, u_{sp}]$ is the optimal operating point, obtained from the previous, steady-state design step, which remains fixed during the controllability assessment and W_x, W_u are weighing matrices that account for penalisation for any deviations of the optimised operating conditions. The goal of this subproblem can be summarised as follows. Given a set of structural design parameters, that is the column lengths of absorber and the stripper as generated by the stochastic algorithm, a set of optimal operating point from the operating optimisation section (i.e., IPOPT) and a set of process disturbances ε, the minimisation of Eq(3) is to be determined, over the controlled and manipulated variables subject to variable bounds that define the allowable variation of the plant and the model constraints, described as a function of the disturbances. The latter are discretised for a wide range of possible disturbance values within predefined limits $[\varepsilon_{i,ref}, \varepsilon_{i,end}]$, according to the following equation:

$$\frac{\varepsilon_i(\zeta) - \varepsilon_{i,ref}}{\varepsilon_{i,ref}} = \theta_i \zeta, \qquad (4)$$

where θ_i represents the direction vector of the i-th disturbance component ε_i. The term ζ is chosen to lie within the unity interval and describes the corresponding disturbance magnitude coordinate.

4.3 Technical data

The considered disturbance scenario accounts for a variation up to 3 % of the CO_2 composition in the flue gas flowrate, which represents a realistic type of potential disturbances in an industrial power plant. The manipulated variables are the amine make-up flowrate, the reboiler duty, the cooler and intercooler duties, and the stripper split ratio. The first two are associated with a higher weight than the rest, as being costlier, and a small deviation from their optimal values translates to a higher cost increase in the objective function. The control variables, in descending order of importance, are the percentage of CO_2 captured, the lean stream loading and temperature. The mathematical model consists of a total of 557 design variables, where 50 are held fixed, 505 equality constraints, and 2 inequality constraints. The simulations ran on an Intel Xeon Gold 5120 @ 2.2GHz computer consisting of 28 physical cores (56 hyper-threads) and 62 GB of memory on GNU/Linux (Ubuntu 18.04 x86-64) operating system. The computational code is written in Fortran and compiled using the Open MPI (2.1.1) implementation of the Message Passing Interface (MPI) protocol.

5. Results and discussion

5.1 Acceleration due to parallelisation

This section discusses computational results, while the next section discusses the quality and economical insights of the obtained solutions. To compare the acceleration obtained from increasing the number of cores, we consider two different simulation cases: case (a) with 20 cores (40 threads) and case (b) with 28 cores (56 threads). The remaining input parameters are kept the same. In both cases, the SA algorithm reached the same optimum solution point, with $F_{obj} = 11.68$, as depicted in Figure 3. However, in case (b) as shown in Figure 3b where more cores are used, the algorithm starts converging to the optimum denoted by a flat line in the objective function value by iteration 1,800, compared to case (a) where the flat line appears after approximately iteration 3,600. The termination criteria are also satisfied earlier in case (b), at iteration 4,800, compared to iteration 6,300 of case (a). The CPU time required in case (b) is 39,818 s (11 h), whereas if the problem was solved in a single thread it would need approximately 63 CPU h. This result strengthens the argument for implementing a parallel framework, which is very efficient in quickly identifying the optimum solution point as fewer iterations have a direct impact on the total time needed by the application. Furthermore, as the number of computational units increases, more process flowsheet designs and operating realisations are tested and this improves the quality of the solution.

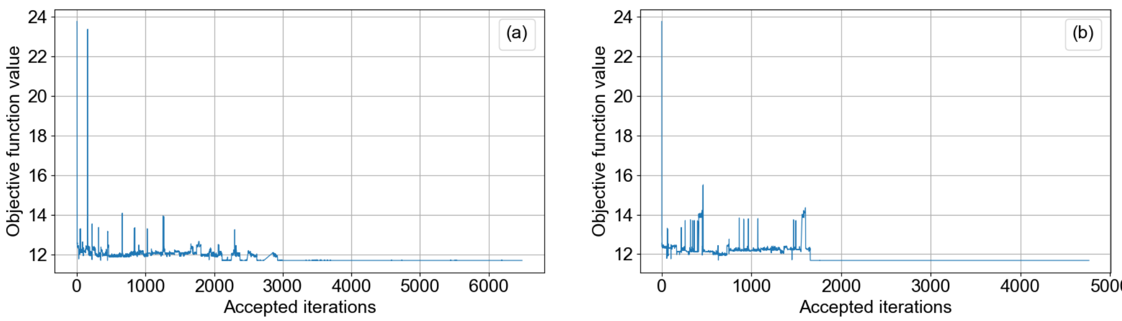

Figure 3: Global optimum solution point obtained by simulated annealing algorithm (a) 20 cores, (b) 28 cores.

5.2 Sequential vs. simultaneous process design and controllability assessment

Table 1 illustrates results between the proposed simultaneous design approach, Case A (combining SA+IPOPT+PITCON) and a conventional, sequential one, Case B. The latter employs only IPOPT as the overall process design algorithm, identifies an optimum process configuration without considering disturbances and is then followed by PITCON to evaluate the controllability performance of the proposed steady-state design. The starting point, the variable bounds and all the input simulation parameters are kept the same in both approaches. The results show that the solution from Case A is improved by about 52 % in terms of overall performance, compared to Case B. The main advantage of Case A is that the simultaneous consideration of the controllability assessment as part of process design (and not as an afterthought as in the sequential case) is able to identify a design which is both robust to disturbances and economically optimum. The solution of Case A indicates that a larger absorption column size (5 stages) and solvent flowrate (25 t/y) are chosen to alleviate the effects of disturbances. Furthermore, the solution proposed in Case A saves 156 MWh/y in reboiler duty and 232 MWh/y in overall cooling.

Table 1: Comparison of the design optimisation results between the two approaches, Case A: SA+IPOPT+PITCON, Case B: IPOPT+PITCON.

Case	A/ Optimum design	A/ setpoint deviation	B/ Optimum design	B/ setpoint deviation	Improvement of A compared to B
CO_2 capture (%)	90.0	0.0	90.0	0.0	-
Lean loading (mol CO_2/mol amine)	0.25	0.0	0.25	0.0	-
Rich loading (mol CO_2/mol amine)	0.53	0.0	0.48	0.0	0.05
Absorber / Stripper length (m)	29 / 24	-	24 / 23	-	-
Reboiler temperature (K)	387.8	0.0	387.5	0.0	-
Reboiler duty (MWh/y)	43,064	785	43,220	728	156
Cooler duty (MWh/y)	12,045	288	11,810	135	232
Intercooler duty (MWh/y)	7,835 / 6,132	155 / 108	8,302 / 6,132	240 / 147	
Solvent make-up flow (t/y)	201.509	0.034	176.145	0.90	-25.364
Absorber bottom pressure (kPa)	147.2	-	121.7	-	-
Stripper bottom pressure (kPa)	158.0	-	156.3	-	-
Stripper split ratio (%)	0.9	0.0	3.5	0.0	-
Objective function value (-)	11.68	-	23.99	-	-

Table 2 lists two different scenarios regarding the operating conditions of the previous cases. In particular, in the first scenario, it is assumed that the process is operating at the optimum design point for half of the total time while the other half of the time it is operating off-design, under the influence of disturbances. In the second scenario, a more frequent shift from the optimal design is investigated. In this case, the process is operating 80 % of the total time under disturbances and only for the remaining 20 % of the time at the optimum design point. In each strategy, the disturbance level is chosen to be normally distributed over its respected time span. In both strategies, the solution proposed in Case A continues to yield lower reboiler duty and total cooling duties compare to Case B, as in the case where no disturbances are present. However, the process operates for a long period of time at an off-design point or equivalently as the disturbance level grows, a clear downwards trend of the aforementioned duties is observed. The same declining trend holds for the solvent make-up flowrate for Case A and B in both scenarios but it decreases at a much lower rate compared to the reduction rate of reboiler duty and overall cooling duties.

Table 2: Comparison of the off-design operation between the two approaches, Case A: SA+IPOPT+PITCON, Case B: IPOPT+PITCON.

Case	A/ 50 % of time off-design	B/ 50 % of time off-design	Improvement of A compared to B	A/ 80 % of time off-design	B/ 80 % of time off-design	Improvement of A compared to B
Reboiler duty (MWh/y)	43,260	43,402	142	43,378	43,511	133
Cooler duty (MWh/y)	12,115	11,843	225	12,158	11,863	191
Intercooler duty (MWh/y)	7,874 / 6,159	8,362 / 6,168		7,898 / 6,175	8,398 / 6,191	
Solvent make-up flow (t/y)	201.514	176.369	-25.145	201.517	176.503	-25.014

6. Conclusions

In the present work, a parallel computational framework for the simultaneous process synthesis of absorption/desorption processes for post-combustion CO_2 capture alongside with a nonlinear sensitivity analysis and controllability assessment is proposed. A generic superstructure with a double section stripper and intercooled absorber modelled after the OCFE formulation to describe the process flowsheet is employed. The optimisation approach consists of a parallel synchronous variation of Simulated Annealing to manage the structural parameters, a nonlinear interior-point algorithm responsible to yield a local optimum point and a nonlinear predictor-corrector continuation method to evaluate the effects of the disturbances. Optimisation results showed the efficiency of the parallel framework, firstly because the obtained economic performance is much better than that of a conventional approach and secondly because the parallelisation of the stochastic algorithm proved time-efficient allowing the investigation of multiple design options at the same time. A limitation of this work is that the controllability assessment is emulated as a series of steady-state process simulations under various disturbance scenarios. The use of dynamic process models could improve the controllability assessment. The optimisation framework can be extended by allowing the SA to handle other parameters. Moreover, various code optimisation and approximate computer techniques can be applied to further reduce the execution time.

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