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Modified coordinate descent methodology for solving process design optimization problems: Application to natural gas plant☆

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ABSTRACT

A modified form of Coordinate Descent methodology (MCD) is presented for solving process optimization problems. The modifications made to the conventional coordinate descent algorithm include search initialization inspired by a pattern search, sequential coordinate randomization for exploring search space and box search for refining of local optimum. The performance of the proposed MCD methodology was examined on benchmark mathematical test problems. After successful convergence of the test problems in reasonable time the MCD algorithm was exploited for the optimization of Natural gas (NG) liquefaction process plant developed in a commercial simulator. The newly developed Korea Single Mixed Refrigerant (KSMR) process was optimized for compression energy demand which is a strong function of refrigerant composition and its operating pressures. MCD was successful in finding the optimum refrigerant composition and operating pressures levels that results in energy savings of 40% and 11% compared with the representative base cases. The suitability of MCD algorithm for NG process plant was further demonstrated by comparing the results of KSMR process with PSO and NSGA-II algorithm. The comparison results demonstrate a nominal improvement in terms of energy savings however the calculation time and ease of implementation and independence of MCD on parameters give it clear advantage. Thus is suitable for solving process design optimization problems particularly related NG plant.

1. Introduction

From the initial design stage, there is considerable room for improvements. Therefore, optimization problems can be found in almost all areas of engineering. In chemical engineering, the typical optimization problems arise in process design (Biegler and Grossmann, 2004) process control (Skogestad, 2000), scheduling (Xu et al., 2012) (Dogan and Grossmann, 2008), process intensification (Khan et al., 2013b), and real-time optimization (Groetschel et al., 2001). Chemical engineering problems are often coupled in terms of the process interactions and complex economics. Hence, an optimal solution through mere intuitive reasoning is unlikely. Therefore, optimization has become the key tool enabling profitable decision making to remain competitive in the chemical industry (Grossmann and Biegler, 2004).

The increase in computational capabilities has resulted in the evolution of an optimization methodology from mere academic interest to a technology with great impact in the process industry (Harjunkoskia et al., 2014). This has led to the development of a number of classes of optimization problem types along with their solution strategies. Lorenz et al. performed a critically annotated review of optimization techniques, particularly in the field of process system engineering (Biegler and Grossmann, 2004). They concluded that over the previous decades, the problems in the process industries mostly were solved using sequential and simultaneous methods. Sequential quadratic programming (SQP) was the most common solver used for Non-linear programming (NLP) problems (Himmelblau, 1972) and the Newton step with Karush–Kuhn–Tucker (KKT) condition was used for rapid convergence. Nevertheless, SQP performs well with smooth continuous convex functions but performs poorly with increasing system nonlinearity, i.e. the abundance of local minima and maxima, because the correct derivatives and gradient are difficult to obtain. The problems associated with NLP leads to the development of a broad class of derivative fee optimization method. These methods have the advantage of easy implementation and

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little prior knowledge of the optimization problem (Biegler and Grossmann, 2004). Most of these methods are derived from heuristics that naturally spawn numerous variations. A few most widely used derivative free optimization (DFO) methods are: Genetic algorithms (Holland, 1992), simulated annealing (Laarhoven and Aarts, 1989), differential evolution (Storn and Price, 1997), and particle swam optimization (Kennedy and Eberhart, 1998). They are best suited for unconstrained problems but the constraint can be handled using penalty function methods (Efrén, 2009) (Khan and Lee, 2013). The performance of DFO methods degraded with increasing number of decision variables, and with no rigorous convergence criterion, the optimal results are always suspect. These methods are rarely applied to the problems with more than few dozen variables (Biegler and Grossmann, 2004). With the advent of parallel computing the DFO optimization approach can be easily adapted to parallel computing and tailored to the number of available processors (Torczon, 1991). Moreover DFO methods with no rigorous termination criteria (based on gradient and stationary points) favor global search. Thus inspired by the above mentioned attributes of DFO methods, in this study the coordinate descent methodology (Wu and Lange, 2008) a version of DFO methods is modified for process system optimization problems. The coordinate descent methodology is based on the idea that the minimization of a multi variable function can be achieved by minimizing it one direction at a time. Once a search direction (after random search) is obtained, a line search utilizing one coordinate at a time is performed, and the search is cycled through each coordinate in sequence. Therefore, each cycle will have used n (decision variables) iterations for each n search direction (Venkataraman, 2009). After obtaining the minimum value of the objective with the defined step size, the same search is followed with a small step size in a narrow space or so called box space within the vicinity of the obtained minimum. Once a locally optimal solution is obtained, the first coordinate point is randomized and the others remain fixed. The same algorithm is followed until the next optimal point. After obtaining the second locally optimal point, the second coordinate point is randomized and the same search steps are followed. Therefore, a number of locally optimal solution arrays are obtained, and the search is terminated after obtaining the defined number of repetitive results within the function tolerance.

The exploited modified coordinate descent (MCD) methodology was verified on a range of standard test problems and after satisfactory performance on test functions (see Section 5) was finally applied for the optimization of KSMR process. The operational parameter optimization of newly developed so-called Korea Single Mixed Refrigerant (KSMR) natural gas liquefaction cycle. The details of the considered KSMR process are mentioned in Section 7. In fact, the MCD methodology was developed to address the optimization problem encountered in the NG processing cycle, including the operation of an NG liquefaction plant, which was rather challenging using traditional optimization approaches (Nogal et al., 2008). When the model development of NG plant is performed in commercial simulator the calculation of gradient information is proportional to the computational complexities of the values of corresponding function (Nesterov, 2012) thus application of MCD which is 'quick and dirty' is well-suited for studied problems where problems are solved under optimization-simulation framework (Aspenlund et al., 2010).

Tough environmental regulations, intense competition and strong growth predictions of the NG market (Annual Energy Outlook, 2013) make optimization of the NG processing cycle an industrially important problem. The failure with the traditional optimization schemes paves the way for the development of customized optimization schemes, such as MCD, which best suits the optimization problem faced in the NG processing cycle and perform well for other numerical test problems.

The remainder of this article is organized as follows. Section 2 gives a theoretical description of MCD. Section 3 compares the results using standard test problems. The problem definition of an NG processing plant is followed by the optimization results/discussion and conclusions.

2. Theoretical description of proposed MCD methodology

The proposed MCD method was based on the idea that the optimization of any multivariable function is performed by minimizing the objective function along one coordinate at a time (Venkataraman, 2009). On the other hand, the proposed MCD method is different from CD methodology in obtaining a local optimal solution and randomizing the search after obtaining a local solution. The proposed methodology begins by choosing a random candidate solution of the decision variables given by Eq. (1) as the initial starting point (Li and Rhinehart, 1998):

$$X_0 = \left\{x_1^0, x_2^0, \ldots, x_n^0\right\}^T \tag{1}$$

To obtain the search direction within the vicinity of the starting point, a sufficiently small step size Δx_i is prescribed in each of the coordinate directions$u_i, i = 1, 2, \ldots, n$. Obtaining an optimal solution depends strongly on the step size selection because a small step size can linger in local points, whereas a large step size can miss a potential solution (Srinivasan et al., 2008). Utilizing the provided step size, and randomly chosen starting point, X_0, exploratory steps similar to a pattern search are made to find the base point. Once a base point is obtained (see Section 3.1), cyclical iterations are performed through each coordinate individually, minimizing the objective function with respect to the individual coordinate direction. If X^k is given, then the i^{th} coordinate of x_i^{k+1} is given by Eq. (2).

$$x_i^{k+1} = \text{argmin} f_{y \in R}\left(x_i^{k+1}, - - -, x_{i-1}^{k+1}, y, x_{i+1}^{k}, - - -, x_n^k\right) \tag{2}$$

Iteration of all different directions or coordinates is performed cyclically to find the descent direction, which is equivalent to a gradient descent. After performing a line search on all coordinates, a new candidate solution update from X_0 to X_1, $F(X_0) \geq F(X_1)$ is obtained. Assuming X_1 as the new starting point, the coordinate descent search is performed over narrow space or the so called box space with a smaller step size around X_1 to find other more promising solutions in the immediate vicinity of X_1. An imaginary space of given dimensions is created around $X_1$and explored in case the previous search overlooked some potential solution to ensure the optimum within the box space with the given step size. After obtaining the locally optimal solution$f(X_1')$, an update from$f(X_1)$, the first coordinate of $X_1'(rand, 2, 3, \ldots., n)$ is randomized while fixing the others to their previous obtained optimal values. The coordinate descent search is performed using $X_1'(rand, 2, 3, \ldots., n)$ as the new starting and optimal space around X_2 is further explored in box space to obtain a new optimal solution, X_2'. This time, the second coordinate of $X_2'(1, rand, 3, \ldots., n)$ is randomized and the search moves are made. Therefore, in this manner, a number of locally optimal solutions are obtained. The search is terminated if the same solutions are obtained repetitively within function tolerance. The termination criterion is a user defined value. Repetition of the same results requires more computational time,