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Evaluation of two termination criteria in evolutionary algorithms for multi-objective optimization of complex chemical processes

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ABSTRACT

Multi-objective (or multi-criteria) optimization (MOO) is useful for gaining deeper insights into trade-offs among objectives of interest and then selecting one of the many optimal solutions found. It has attracted numerous applications in chemical engineering. Common techniques for MOO are adaptations of stochastic global optimization methods, which include metaheuristics and evolutionary methods, for single-objective optimization. These techniques have been used mostly with maximum number of generations (MNG) as the termination criterion for stopping the iterative search. This criterion is arbitrary and computationally inefficient. Hence, this study investigates two termination criteria based on search progress (i.e., performance or improvement in solutions), for MOO of three complex chemical processes modeled by process simulators, namely, Aspen Plus and Aspen HYSYS. They are Chi-Squared test based Termination Criterion (CSTC) and Steady-State Detection Termination Criterion (SSDTC). Both these criteria are evaluated in two evolutionary algorithms for MOO. Results show that CSTC and SSDTC are successful in giving optimal solutions close to those after MNG but well before MNG. Of the two criteria, CSTC is more reliable and terminates the search earlier, thus reducing computational time substantially.

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1. Introduction

Optimization of the design and operating conditions of industrial chemical plants is essential for improving their performance. In such cases, many optimization problems involve simultaneous minimization and/or maximization of more than one objective related to economics, environment, energy and safety, and some of these objectives can be conflicting in nature. This type of optimization is referred to as multi-objective optimization (MOO), and its resulting optimal solutions are termed as Pareto-optimal front, which consists of many non-dominated solutions or equally good solutions in terms of objectives used. More details on MOO and its various applications in chemical engineering can be found in Bhaskar et al. (2000), Zaman and Rangaiah (2009), Sharma and Rangaiah (2013a), and Rangaiah et al. (2015). Similarities and differences between MOO and Single Objective Optimization (SOO) are also summarized in Rangaiah et al. (2015). Majority of the optimization studies covered in these reviews have used an evolutionary algorithm such as the elitist Non-dominated Sorting Genetic Algorithm (NSGA-II), and they were programmed using programming languages such as FORTRAN and C++.

Although FORTRAN and C++ are used by researchers and engineers, they are more familiar with Microsoft Excel (MS Excel), which is widely used in both industry and academia. Hence, Sharma et al. (2012) implemented binary-coded NSGA-II algorithm in MS Excel (Excel-based MOO or EMOO program), to provide a user-friendly and readily available platform for performing MOO. An MOO problem can also be solved by deterministic optimization methods by first transforming it into a SOO problem, which is known as scalarization approach (Rangaiah et al., 2015). The resulting SOO problem has to be solved repeatedly for obtaining many non-dominated solutions. For example, ε-constraint method

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(belonging to the scalarization approach) was employed for deployment of a hydrogen supply chain (Almaraz et al., 2015), for optimization of forest-based biorefinery supply chains (Cambero et al., 2016), and for design and retrofitting of water networks (Sharma and Rangaiah, 2016).

Evolutionary algorithms such as genetic algorithms and differential evolution, and other stochastic algorithms (e.g., teaching–learning based optimization) for MOO have been implemented and used with maximum number of generations (MNG) or maximum number of function evaluations (i.e., computational effort) as the termination criterion for stopping the search (e.g., Sharma et al., 2012; Patel and Savsani, 2014; de Faria et al., 2016; Patel and Padhiyar, 2017). In order to ensure that optimal solutions are found, a large MNG has to be chosen; moreover, suitable MNG will change from one run to another owing to the stochastic nature (arising from the use of random numbers) in evolutionary/stochastic algorithms. Hence, use of MNG is computationally inefficient for application problems, which require computational time of seconds to minutes for each evaluation of objective functions and constraints. There is a need for reliably terminating the search by the evolutionary algorithm right after convergence (i.e., not much improvement in the optimal solutions over a number of generations).

For MOO, Trautmann et al. (2008, 2009) proposed a termination criterion using different performance metrics to monitor search progress; search is terminated if variations in the performance metrics are not significant over certain number of generations. Sharma and Rangaiah (2013b) developed an improvement-based search termination criterion, and used it in Multi-Objective Differential Evolution (MODE). After analyzing several performance metrics, they chose Generational Distance (GD) and Spread (SP) for implementing the Chi-Squared (χ^2) test based Termination Criterion (CSTC) in Improved MODE (IMODE) program. They tested CSTC on constrained benchmark problems and then on alkylation, Williams-Otto and fermentation processes. Guerrero et al. (2010) proposed least square termination criterion, which utilizes mutual domination rate, hyper volume and epsilon indicator. Recently, Saxena et al. (2016) summarized the approaches for termination criterion used in around 10 papers, mostly from conferences, and identified their limitations. Then, they proposed an entropy-based termination criterion and evaluated its performance through extensive simulations. Abdul Kadhar and Baskar (2016) proposed a termination criterion based on variations of Tchebycheff objective, for use in decomposition-based evolutionary algorithms for MOO. After testing on benchmark problems, they assessed the stopping criterion on the optimal design of a PID controller for both stability and performance.

Rhinehart (2014) proposed and tested a convergence criterion for SOO based on steady-state detection by comparing the objective function variance estimated using two different methods. For MOO, Wong et al. (2016) developed Steady-State Detection Termination Criterion (SSDTC) using GD, and implemented it in the EMOO program (having both real- and binary-coded NSGA-II). Then, they employed this program with both CSTC and SSDTC to solve mathematical test functions and shell-and-tube heat exchanger design problems. Results reported in Sharma and Rangaiah (2013b) and Wong et al. (2016) show the potential benefit of CSTC and SSDTC. However, these two promising termination criteria have not been applied and tested for MOO of complex chemical processes simulated with a process simulator such as Aspen Plus and Aspen HYSYS. Further, SSDTC has been used in the EMOO program only, and not in the IMODE program.

Hence, the broad objectives of this study are to evaluate the effectiveness of CSTC and SSDTC for MOO of complex chemical processes simulated using a process simulator, and to assess the applicability of CSTC and SSDTC in two evolutionary algorithms. For this study, Dividing-Wall Column (DWC) design, cumene production process, and biodiesel production process are optimized using both EMOO and IMODE programs having CSTC and SSDTC besides MNG as termination criteria. Effectiveness of these two termination criteria in both EMOO and IMODE programs is evaluated. Results of this study show the benefit of CSTC and SSDTC for MOO of chemical processes independent of process simulator and evolutionary algorithm employed. Significant contribution of this study is comprehensive evaluation of two alternate search termination criteria in two MOO algorithms/programs on three chemical processes simulated using commercial simulators.

The next section briefly describes EMOO and IMODE programs as well as the two termination criteria (CSTC and SSDTC). Section 3 provides details on the assessment of the two termination criteria and the two MOO programs for DWC design, cumene production process and biodiesel production process, respectively. Conclusions for this study are provided in the final section.

2. Multi-objective optimization and termination criteria

The two MOO algorithms with termination criteria were coded using Visual Basic for Applications (VBA) in MS Excel. Further, MS Excel worksheets were used as user interface for providing the input and getting the results. See Sharma et al. (2012) and Sharma and Rangaiah (2013b) for algorithm and details of EMOO and IMODE programs, respectively. The main differentiating factor between the two programs is the MOO algorithm; EMOO is based on NSGA-II (Deb et al., 2002) whereas IMODE is based on differential evolution with taboo list (Srinivas and Rangaiah, 2007). In IMODE, taboo list allows for reduction in computational time by skipping (i.e., without evaluating) generated individuals that are close to previously evaluated individuals.

Values of algorithm parameters in EMOO and IMODE are as follows (Sharma and Rangaiah, 2013b; Wong et al., 2016). Population size of 100 and maximum number of generations of 150 are used in both the programs. Other choices in EMOO are as follows: real coding, simulated binary crossover (SBX) with probability of 0.5, non-uniform mutation with probability of 0.01 and tournament selection. In IMODE, initial value for both crossover probability and mutation factor is 0.5, and both these are self-adapted during the search. These parameter values/choices in EMOO and IMODE are kept the same for solving three chemical processes presented later, in order to test their robustness. There are several inequality constraints in the formulated MOO problems for all three case studies. These inequality constraints are handled using the feasibility approach (Deb et al., 2002), which has been successfully used in a wide range of problems by many researchers.

Performance-based termination criteria require suitable metrics for monitoring the progress or improvement in the optimal solutions. In the case of SOO, the objective function value can be used for this. In the case of MOO, there are usually many non-dominated (optimal) solutions, and all of them need to be assessed using suitable performance metrics. After analyzing a number of performance metrics, Sharma and Rangaiah (2013b) chose GD and SP based on their effectiveness to monitor the convergence and distribution of non-dominated solutions, and for their computational simplicity.

Usually, GD is used to check the convergence of non-dominated solutions obtained to the true Pareto-optimal front (van Veldhuizen and Lamont, 1998). Since true Pareto-optimal front is yet to be found in applications, Sharma and Rangaiah (2013b) modified GD to avoid using the true Pareto-optimal front by calculating it based on non-dominated solutions obtained from two consecutive generations. Modified GD, GD_m, is calculated as follows:

$$d_i = \min\|S_i - S_j\|_2 \text{ with respect to } j=1,2,\ldots,N_{curr} \quad (1)$$

$$GD_m = \frac{1}{N_{prev}}\sqrt{\sum_{i=1}^{N_{prev}} d_i^2} \quad (2)$$

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