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A Comparative Study of Differential Evolution Algorithms for Estimation of Kinetic Parameters

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Abstract

The problem of estimating kinetic parameters in dynamic models is important and even more difficult than with algebraic models. The solution of these types of problems is usually very difficult due to their highly nonlinear, multidimensional and multimodal nature. This paper presents a comparative study of Differential Evolution (DE) algorithms for solving such problems. In this work, two modified versions of DE algorithm [called Modified Differential evolution (MDE) and Trigonometric Differential Evolution (TDE)] are used to solve kinetic parameter estimation problems from chemical engineering field. The computational efficiency of MDE algorithm is compared with that of DE and TDE algorithms. Results indicate that performance of MDE algorithm is better than that of DE and TDE algorithms.

Key words: Kinetic parameter estimation; Optimization; Evolutionary algorithm; Differential Evolution; Dynamic models.

1. INTRODUCTION

Parameter estimation is a key step in the development of mathematical models of physical phenomena and the problem of estimating parameters in dynamic models is important and even more difficult than with algebraic models. The extra difficulty arises from the inclusion of nonlinear differential-algebraic equations in the optimization problems. This type of problems arises most often in the estimation of kinetic constants from experimental time series data [Floudas et al., 1999].

In general, there are two types of approaches to address the parameter estimation problem for such dynamic systems. Both, the *sequential* and *simultaneous* approaches of dynamic optimization have been widely studied in this context [Michalik et al., 2009]. In either approach, the objective is to minimize a weighted squared error between the observed values and those predicted by the model [Lin and Stadtherr, 2006]. The key idea is to estimate an unknown parameter vector $p = (p_1,...,p_n)^T$ of a mathematical model that describes a real-life situation, by minimizing the distance of some known experimental data from theoretically predicted values of a model function at certain time values [Schittkowski, 2007]. Thus, kinetic parameters of model that cannot be measured directly also can be identified by a least squares fit and analyzed subsequently in a quantitative way.

The solution of these types of problems is usually very difficult due to their highly nonlinear, multidimensional and multimodal nature. In fact, several deterministic techniques [Esposito and Floudas, 2000; Gau and Stadtherr, 2000; 2002; Papamichail and Adjiman, 2004; Tang, 2005; Lucia et al., 2005; Lin and Stadtherr, 2006; Schittkowski, 2007; Michalik et al., 2009] have been proposed to solve these problems but difficulties related to ease of implementation, global convergence, and good computational efficiency have been frequently found.

Nowadays, evolutionary algorithms have become popular for solving problems of highly nonlinear, multidimensional and multimodal nature, in various science & engineering disciplines. Differential Evolution [Storn and Price, 1995] is one such algorithm. DE algorithm has been applied to solve several types of problem (nonlinear, mixed integer nonlinear, dynamic optimization) encountered especially in chemical engineering [Wang and Chiou, 1997; Chiou and Wang, 1999; Angira, 2005; Angira and Babu, 2006; Angira and Alladwar, 2007]. Also, a detailed review of the basic concepts of DE and its application to many types of problems and the theoretical studies conducted on DE so far is presented in literature [Das and Suganthan, 2011].

Recently, a modified version of DE named Modified Differential Evolution (MDE) was proposed [Angira and Babu, 2005]. But the application of DE or MDE to solve kinetic parameter estimation problem in open literature is scarce [Liu and Wang, 2009; Babu and Sastry, 1999; Angira, 2011]. This paper presents the application and performance evaluation of MDE for solving problems of estimating kinetic parameters in nonlinear dynamic models of chemical engineering processes. Numerical results are compared with that of obtained using DE and TDE algorithms. Details of the DE, TDE and MDE algorithms are avoided for the sake of brevity and the reader may refer to literature [Fan and Lampinen, 2003; Angira, 2005; Angira and Babu, 2006; Babu and Angira, 2006] for the same. This paper is organized as follows. Test problems are described briefly in Section-2. Results and discussion are presented in Section-3 followed by conclusions in Section-4.

2. TEST PROBLEMS

2.1. A First-Order Irreversible Liquid-Phase Reaction

This example is a parameter estimation problem with two parameters and two differential equations in the constraints. It appears in literature [Tjoa and Biegler, 1991; Floudas *et al.* 1999; Esposito and Floudas, 2000]. It involves a first-order irreversible isothermal liquid-phase chain reaction: $A \xrightarrow{k_1} B \xrightarrow{k_2} C$. The problem can be formulated as follows:

Objective function: $$\underset{k_1,k_2}{Min} \quad J = \sum_{\mu=1}^{10}\sum_{j=1}^{2}\left(x_{\mu,j} - x_{\mu,j}^{\exp}\right)^2 \tag{4}$$

Subject to constraints:

$$\frac{dx_1}{dt} = -k_1 x_1 \tag{5}$$

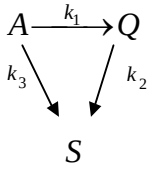
$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 \tag{6}$$

Initial conditions: $$x_1(t=0) = 1 \quad \text{and} \quad x_2(t=0) = 0; \tag{7}$$

Variable bounds are: $0 \le k_1, k_2 \le 10$, t_f = 1.0, and x_1, x_2 are the mole fractions of components *A* and *B*, respectively. k_1 and k_2 are the rate constants of the first and second reaction, respectively. $x_{\mu,j}^{\exp}$ is the experimental point for the state variable *j* at time t_μ. The experimental points are taken from literature [Floudas *et al*., 1999].

2.2. Catalytic Cracking of Gas Oil

This parameter estimation test problem consists of three parameters and two differential equations in the constraints. It appears in literature [Tjoa and Biegler, 1991; Floudas *et al.*, 1999; Esposito and Floudas, 2000]. It involves an overall reaction of catalytic cracking of gas oil (*A*) to gasoline (*Q*) and other side products (*S*):



This reaction scheme involves nonlinear reaction kinetics rather than the simple first-order kinetics in the previous test problem. Only the concentrations of *A* and *Q* were measured; therefore, the concentration of *S* does not appear in the model for estimation. The problem can be formulated as follows:

Objective function $$\underset{k_1,k_2,k_3}{Min} \quad J = \sum_{\mu=1}^{20}\sum_{j=1}^{3}\left(x_{\mu,j} - x_{\mu,j}^{\exp}\right)^2 \tag{13}$$

Subject to constraints $\frac{dx_1}{dt} = -(k_1 + k_3)x_1^{\,2}$ (14)

$$\frac{dx_2}{dt} = k_1 x_1^{\,2} - k_2 x_2 \quad (15)$$

Initial Conditions $x_1(t=0) = 1$; and $x_2(t=0) = 0$; (16)

Variable bounds are $0 \le k_1, k_2, k_3 \le 20$, t_f = 0.95, and x_1, x_2 are the mole fractions of components *A* and *Q*, respectively. k_1, k_2 and k_3 are the rate constants of the respective reactions. $x_{\mu,j}^{\exp}$ is the experimental point for the state variable *j* at time t_μ. The experimental points are taken from literature [Floudas *et al.,* 1999].

3. RESULTS & DISCUSSIONS

For the numerical solution of the above test problems, each continuous problem is transformed into a finite-dimensional nonlinear programming problem using state parameter discretization (known as the sequential approach). Here the state parameters are discretized in to *D* stages of known experimental state variable data. Differential equations are integrated using Runge-Kutta 4th order method, in each *D* stage so as to evaluate the objective function and the constraints.

For each test problem, 50 different simulation runs of each DE, MDE and TDE algorithms are carried out. Algorithms are coded in C language. The reported results of this study are obtained using an IBM computer (Pentium-IV/3.2 GHz). Termination criteria used is $\lfloor \max - \min \rfloor \le 1 \times 10^{-12}$ (where *max* and *min* is best and worst objective function values respectively).

3.1. A First-Order Irreversible Liquid-Phase Reaction

For this kinetic parameter estimation problem, the key parameters of DE, MDE and TDE are taken as *F* = 0.5, *CR* = 0.8, M_t = 0.9, *NP* = 10**D*. Table-1 shows the highest, average and lowest fractional difference of 50 different runs of each algorithm. The fractional difference (f_d) is given by $f_d = 1 - J / J_{best}$ where J_{best} is the best objective function value reported in literature [Floudas et al., 1999] and *J* is obtained objective function value. For this test problem $J_{\text{best}} = 1.18584 \times 10^{-06}$. It is found that f_d value is same for all algorithms and for all 50 runs. The precision of results is quantified by standard deviation of zero for all three algorithms.

Table-2 shows comparison of results of all three algorithms. From Table-2, it is clear that all three algorithms are converging to same global optimum value. The CPU-time required to obtain global optimum using MDE is less than that of DE and TDE algorithm. MDE takes approximately 17% less CPU-time as compared to DE & TDE algorithms. The CPU-time required to obtain global optimum using TDE algorithm is nearly same as that required by DE.

Table-1. Fractional difference variation for Test Problem-2.1.

Algorithm	Fractional difference (f_d)		
	Highest	Average	Lowest
DE	-4.2×10^{-06}	-4.2×10^{-06}	-4.2×10^{-06}
MDE	-4.2×10^{-06}	-4.2×10^{-06}	-4.2×10^{-06}
TDE	-4.2×10^{-06}	-4.2×10^{-06}	-4.2×10^{-06}

Table-2. Comparison of Results for Test Problem-2.1.

Algorithm	Best Objective function value (J) obtained	CPU time (s)
DE	1.185845×10^{-06}	0.40
MDE	1.185845×10^{-06}	0.33
TDE	1.185845×10^{-06}	0.39

The global optimum parameters (corresponding to true global optimum objective function value) obtained are same for each algorithm, which are k_1 = 5.003487, and k_2 = 1.0. The experimental data points and the obtained data points (for a typical run) for state variables are shown in Fig. 1 & 2. From Fig. 1 & 2, it is clear that obtained state variable data is matching with that experimental data and as reported in literature [Floudas et al., 1999; Esposito & Floudas, 2000; Papamichail & Adjiman, 2004].

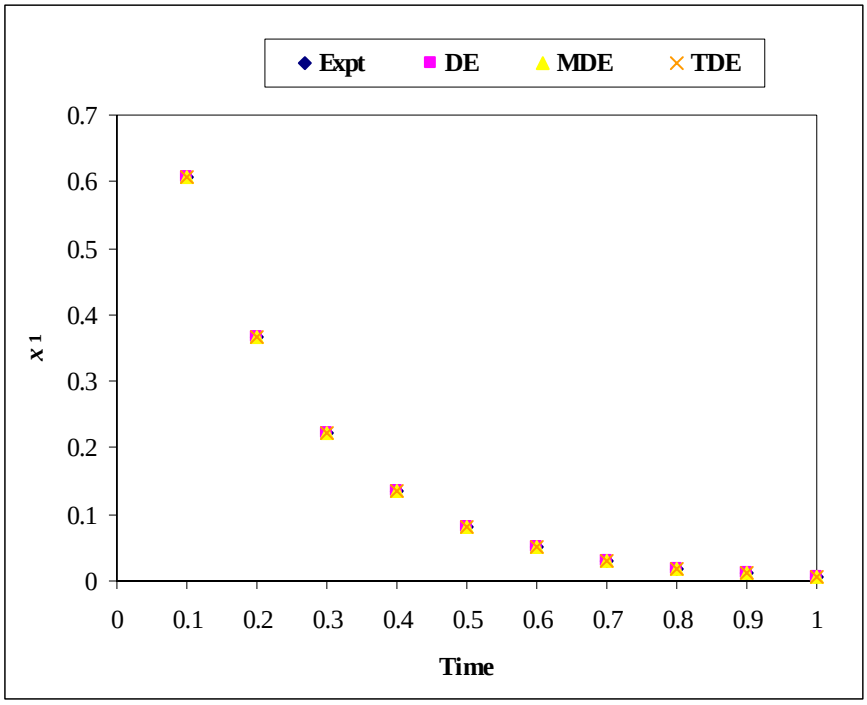


Fig. 1. Experimental data points and obtained data points for state variable (x_1) of Test Problem-2.1.

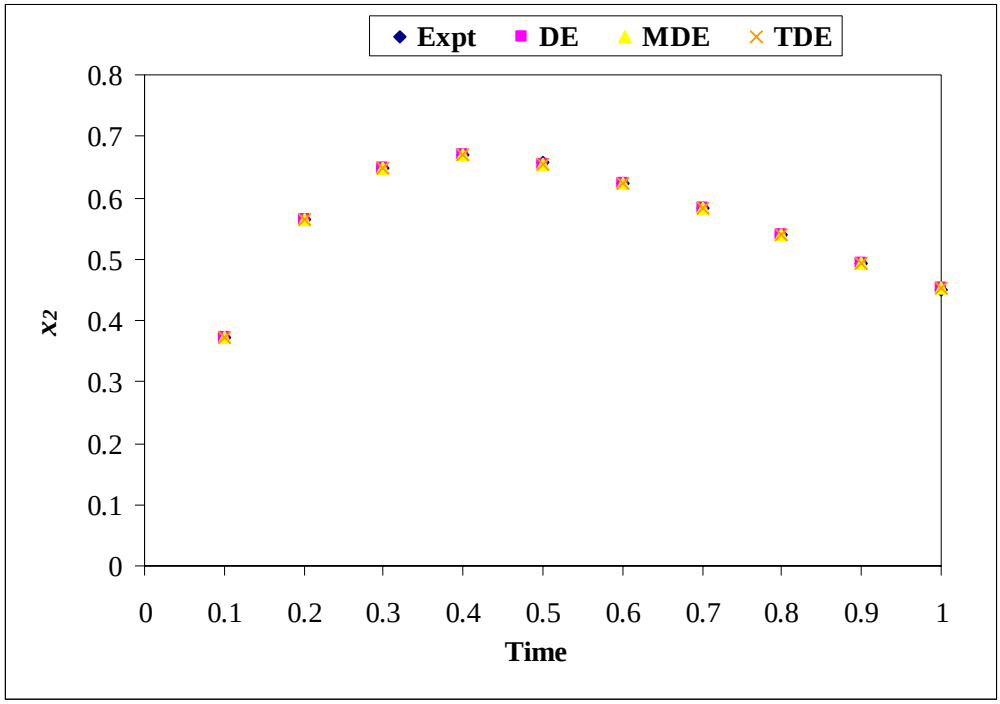


Fig. 2. Experimental data points and obtained data points for state variable (x_2) of Test Problem-2.1.

3.2. Catalytic Cracking of Gas Oil

For this kinetic parameter estimation problem, the key parameters of DE, MDE and TDE are taken as $F = 0.5$, $CR = 0.8$, $M_t = 0.9$, $NP = 10*D$. Table-3 shows the highest, average and lowest fractional difference of 50 different runs of each algorithm. For this problem, $J_{best} = 2.655670\times10^{-03}$. The overall accuracy of 50-f_d values is quantified by their average of 0.000001 for DE and MDE algorithms and an average value of -0.011534 for TDE algorithm as shown in Table-3. The precision of results is quantified by standard deviation of zero for DE and MDE algorithms and 0.038172 for TDE algorithm.

Table-3. Fractional difference variation for Test Problem-2.2.

Algorithm	Fractional difference (f_d)		
	Highest	Average	Lowest
DE	1.0×10^{-06}	1.0×10^{-06}	1.0×10^{-06}
TDE	1.0×10^{-06}	-0.011534	-0.234029
MDE	1.0×10^{-06}	1.0×10^{-06}	1.0×10^{-06}

Table-4 shows comparison of results for all three algorithms. From Table-4, it is clear that all three algorithms are converging to same global optimum value up to eleven decimal places. The CPU-time required to obtain global optimum using MDE is less than DE and TDE algorithm. MDE algorithm takes approximately 19% less CPU-time as compared to DE algorithm. The CPU-time required to obtain the global optimum using TDE algorithm is 48% more as compared MDE algorithm and 36% more as compared to DE algorithm. The global optimum parameters (corresponding to true global optimum objective function value) obtained are same for each algorithm, which are k_1 = 12.21401, k_2 = 7.979833, and k_3 = 2.22162.

Table-4. Comparison of Results for Test Problem-2.2.

Algorithm	Best Objective function value (*J*) obtained	CPU time (*s*)
DE	2.65566×10^{-03}	1.02
TDE	2.65566×10^{-03}	2.27
MDE	2.65566×10^{-03}	0.82

From Fig. 3, it can be observed that for this test problem the TDE algorithm converged into closer vicinity of the global optima while DE and MDE algorithms converged to the true global optima. This suggests that DE & MDE algorithms have better convergence reliability than the TDE algorithm.

The experimental data points and the obtained data points (for a typical run) are shown in Fig. 4 & 5. From Fig. 4 & 5, it is clear that obtained state variable data is matching with that reported in literature [Floudas et al., 1999; Esposito and Floudas, 2000; Papamichail and Adjiman, 2004].

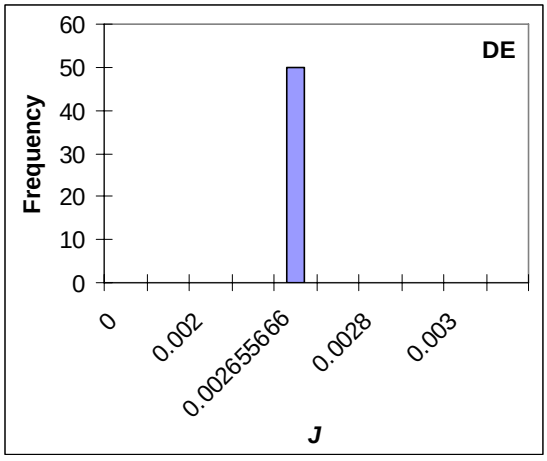


Fig. 3(a). DE algorithm

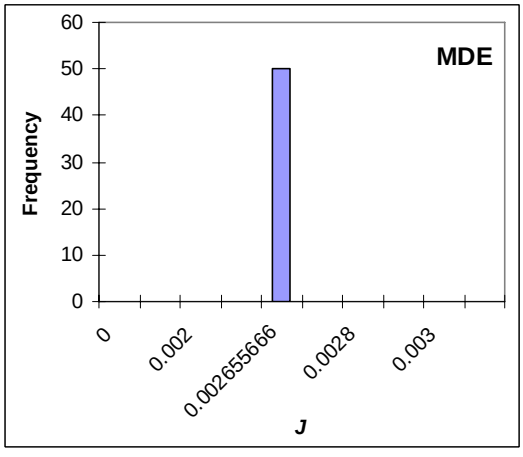


Fig. 3(b). MDE algorithm

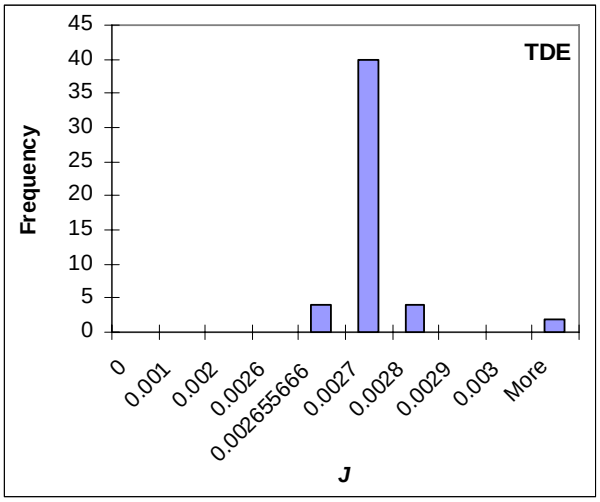


Fig. 3(c). TDE algorithm

Fig. 3. Histograms of the function values obtained by the DE, MDE, and TDE algorithms for fifty independent trial runs for Test Problem-2.2.

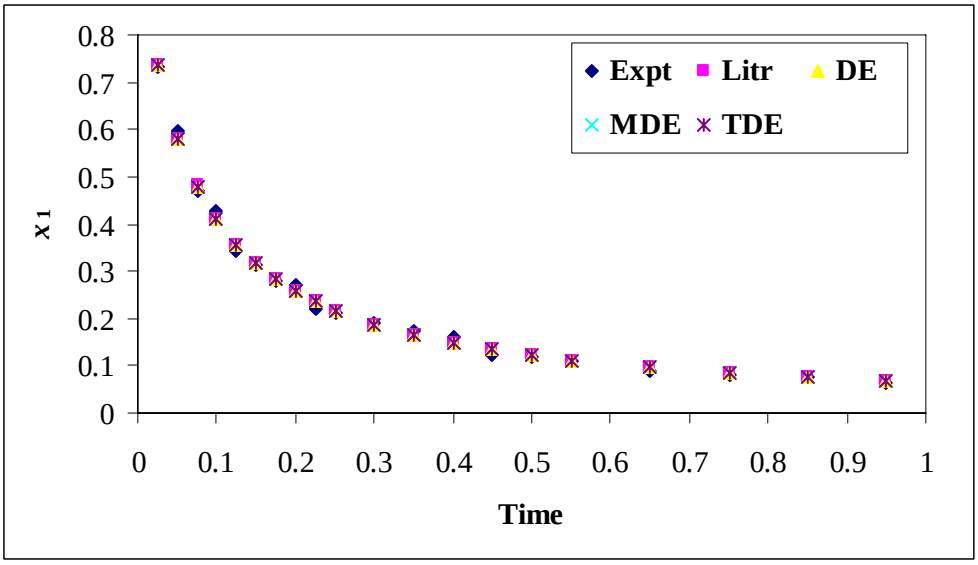


Fig. 4. Experimental data points and obtained data points for state variable (x_1) of Test Problem-2.2.

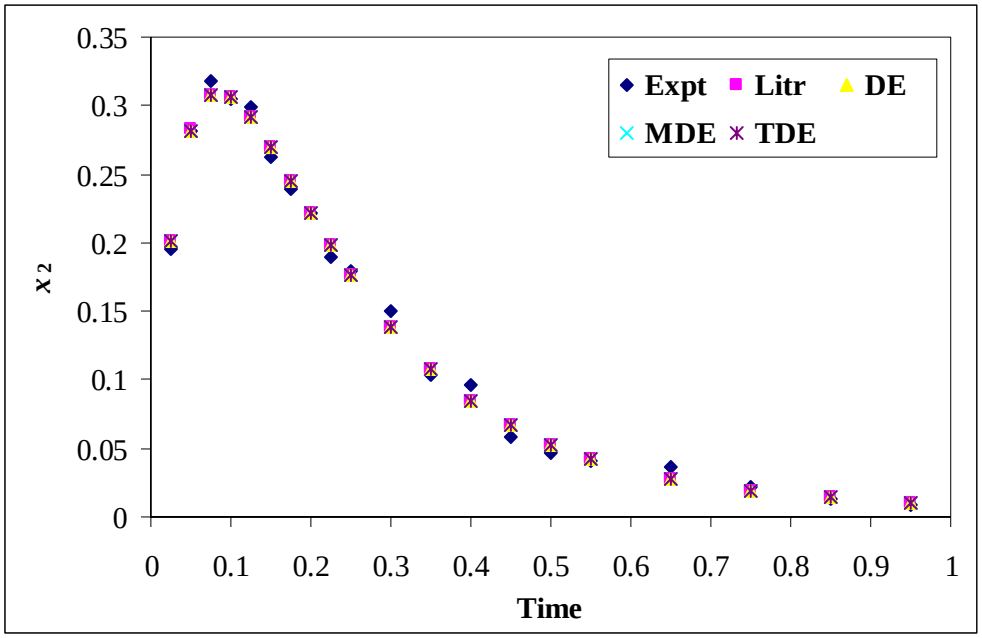


Fig. 5. Experimental data points and obtained data points for state variable (x_2) of Test Problem-2.2

4. CONCLUSIONS

In this paper the performance of DE, TDE, and MDE algorithms is compared for solving problems of estimating kinetic parameters from chemical engineering. The performance of TDE algorithm was found to be worst among the three algorithms used in the present study. The two algorithms (DE and MDE) are able to obtain global optimum with 100% convergence overall the 50 different executions of the each algorithm. But MDE algorithm is found to be efficient and faster than the DE and TDE algorithms for the test problems considered in the present paper.

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