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Kinetic Parameter Estimation Using Modified Differential Evolution

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***Abstract*—** For the development of mathematical models in chemical engineering, the parameter estimation methods are very important as design, optimization and advanced control of chemical processes depend on values of model parameters obtained from experimental data. Nonlinearity in models makes the estimation of parameter more difficult and more challenging. This paper presents an evolutionary computation approach for solving such problems. **In this work, a modified version of Differential Evolution (DE) algorithm [named Modified Differential evolution (MDE)] is used to solve a kinetic parameter estimation problem from chemical engineering field.** The computational efficiency of MDE is compared with that of original DE and Trigonometric Differential Evolution (TDE). Results indicate that performance of MDE algorithm is better than that of DE and TDE.

Keywords - Evolutionary computation; Differential Evolution; Parameter estimation; Dynamic optimization

I. 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 [1].

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 [2]. In either approach, the objective is to minimize a weighted squared error between the observed values and those predicted by the model [3]. The key idea is to estimate **an unknown parameter vector $p = (p_1,...,p_r)^T$ 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 [4]. Thus, model parameters that cannot be measured directly also can be identified by a least squares fit and analyzed subsequently in a quantitative way.

The general formulation of typical parameter estimation problem is given below :

Objective function:

$$\underset{x_\mu,\theta}{Min}\, J = \sum_{\mu=1}^{r}\sum_{i=1}^{m}\left(x_{\mu,i} - x_{\mu,i}^{\exp}\left(t_j\right)\right)^2 \qquad (1)$$

Constraints:

Dynamic model:

$$f\left(\frac{dz}{dt}, z, \theta\right) = 0\,,\, z(t_0) = z_0 \qquad (2)$$

Point Constraints:

$t = t_\mu$; $z_i - x_{\mu,i} = 0$; $i = 1,.....,m$; $\mu = 1,....,r$; (3)

Where f is a system of l differential-algebraic functions which represents the non linear model, z is a vector of i state variables, θ is a vector of p parameters in bounds $p^{LB} \le p \le p^{UB}$, and x_μ is a vector of i fitted data variables at the μ^{th} data point. $t\,\varepsilon\left[t_0, t_r\right]$ and t_μ is the time associated with the μ^{th} observation.

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 [2, 3, 4, 5, 6, 7, 8, 9, and 10] have been proposed to solve these problems but difficulties related to ease of implementation, global convergence, and good computational efficiency has been frequently found. Nowadays evolutionary

algorithms have become popular, for solving problems of highly nonlinear, multidimensional and multimodal nature, in various engineering discipline. Differential Evolution [11] is one such algorithm. Differential Evolution (DE) algorithm has been applied to solve several type of problems (e.g. nolinear, mixed integer nolinear, dynamic optimization) encountered especially in chemical engineering [12, 13, 14, 15, 16 etc. to name a few].

Recently, Angira and Babu [17] proposed a modified version of DE named Modified Differential Evolution (MDE). But the application of DE and MDE to solve parameter estimation problem is scarce in open literature. Earlier, Angira and Alladwar [16] compared the performance of DE and Trigonometric Differential Evolution (TDE) for solving parameter estimation problem encountered in chemical engineering.

This paper presents the application and performance evaluation of MDE for solving problems of estimating parameters in dynamic models. Numerical results are compared with that obtained using DE and TDE. The details of the MDE algorithm are presented in Angira [14], Angira and Babu [15, 17] and Babu and Angira [18]. And the details of TDE algorithm are available in [16, 19, and 20].

II. PROBLEM FORMULATION

This example is a parameter estimation problem with two parameters and two differential equations in the constraints. It appears in [21] as well as in [1, 5, 16 and 20]. 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:

$$\underset{k_1,k_2}{Min} J = \sum_{\mu=1}^{10}\sum_{i=1}^{2}\left(x_{\mu,j} - x_{\mu,j}^{\exp}\right)^2 \qquad (4)$$

Subject to constraints:

$$\frac{dx_1}{dt} = -k_1 x_1 \qquad (5)$$

$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 \qquad (6)$$

Initial conditions: $x_1(t=0)=1$ and $x_2(t=0)=0$; (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 *i* at time t_j. The experimental points used are taken from [1].

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

III. RESULTS & DISCUSSION

For kinetic parameter estimation problem, the key parameters of DE, MDE and TDE are taken as F = 0.5, CR = 0.8, NP = 10D.

For each problem, 50 runs of each DE and TDE algorithms are carried out in order to ensure that the seed used for the random number generator did not bear any influence on the quality of the results obtained. All the algorithms are coded in C language (Microsoft Visual C++ 6.0, compiler). The reported results of this study are obtained using an IBM computer (Pentium-IV/2.40 GHz/RAM 256 MB).

Termination criteria used is $\lfloor \max - \min \rfloor \le 1\times10^{-12}$ (where max and min is best and worst objective function values respectively). The results of 50 different runs of each algorithm are plotted in Fig. 1. The fractional difference (*f*) is given by $f = 1 - J / J_{best}$ where J_{best} is the best objective function value reported in literature [1, 16] and *J* is obtained objective function value. The obtained tuned M_t value of TDE algorithm for this case study is 0.9. In Fig. 1, the overall accuracy of 50-*f* values is quantified by their low average of -0.000004 for all three algorithms. The precision of results is quantified by standard deviation of zero for all three algorithms.

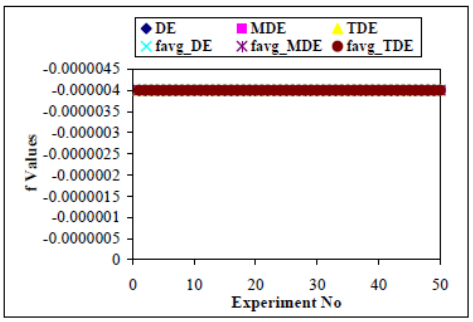

Figure 1. Fractional difference variation

Table-1 shows comparison of results of all three algorithms. From Table-1, it is clear that all three algorithms are converging to same global optimum value up to twelve decimal places. The CPU-time required to obtain global optimum using MDE is less than that of DE and TDE algorithm. MDE is saving approximately 17% CPU-time as compared to DE. The CPU-time required to obtain global optimum using TDE algorithm is nearly same as required by DE.

The global optimum parameters corresponding to optimum objective function value obtained for each run of fifty different runs are same for each algorithm, which are k_1 = 5.003487 and k_2 = 1.00. The experimental data points and the obtained data points are shown in Fig. 2 & Fig. 3. From Fig. 2 & Fig. 3, it is clear that obtained state variable data are matching with that experimental data and as reported in [1, and 8].

TABLE I. COMPARISION OF RESULTS

Algorithm	**Objective function value (*J*)**	**CPU time (*s*)**
DE	1.185845E-6	**0.45**
MDE	1.185845E-6	**0.38**
TDE	1.185845E-6	**0.46**

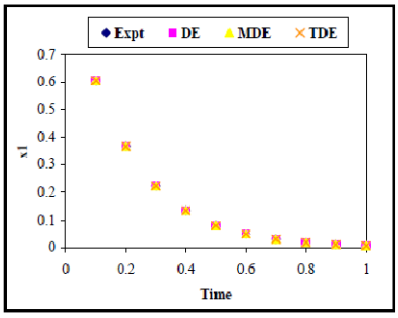

Figure 2. Experimental points and state variable trajectory for x_1

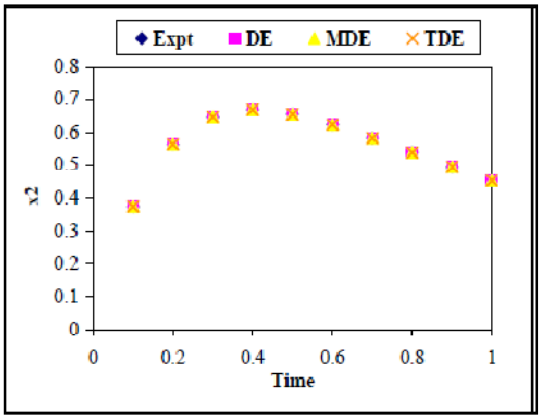

Figure 3. Experimental points and state variable trajectory for x_2

IV. CONCLUSIONS

In this paper the performance of MDE algorithm is evaluated for solving a problem of estimating parameters in dynamic models from chemical engineering. The three algorithms (MDE, DE and TDE) are able to obtain global optimum with nearly 100% convergence overall the 50 different executions of the algorithms. The performance of MDE algorithm is compared with that of DE and TDE. The MDE algorithm is found to be efficient and faster than the DE and TDE algorithms for the problem considered in the present paper. Further, a detailed study is needed to establish the computational efficiency of these algorithms in solving parameter estimation problems.

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