

Optimal Design of an Auto-thermal Ammonia Synthesis Reactor using Differential Evolution

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ABSTRACT

In the present study, the Differential Evolution (DE), an evolutionary computation technique, is applied to the optimal design of an auto-thermal ammonia synthesis reactor. This paper also presents the new concept of "Nested DE" (DE is also used to find out the best combination of key parameters of DE itself). The main objective in the optimal design of an auto-thermal ammonia synthesis reactor is the estimation of the optimal length of reactor for different top temperatures with the constraints of energy and mass balance of reaction and feed gas temperature & mass flow rate of nitrogen for ammonia production. Thousands of combinations of feed gas temperature, nitrogen mass flow rate, reacting gas temperature and reactor length are possible. This paper presents the application of two methods, viz., Runge-Kutta variable step size method, and Gear's method in combination with DE, and verify the contradictory results reported using simple GA in earlier literature. Apart from determining the optimal reactor length, the comparison of results obtained from different methods is presented. DE is found to be a robust, fast and simple evolutionary computation technique for optimization problems.

Keywords: Evolutionary Computation, Optimization, Ammonia Synthesis Reactor, Differential Evolution (DE), Nested DE.

1. INTRODUCTION

Ammonia is one of the most important chemicals produced as it enjoys the wide use in the manufacture of fertilizers. Hence modeling and simulation of ammonia manufacturing process has received considerable attention among the process industries. Simulation models for ammonia synthesis converters of different types have been developed for design & optimization [1, 14, 16, 22, 29, 31], and control [28] purposes.

Upreti & Deb [31] used Murase's formulation with correct objective function and correct stoichiometric expressions of the partial pressures of N_2 , H_2 , and NH_3 . They used simple GA in combination with Gear package of NAG library's subroutine, D02EBF, for the optimization of ammonia synthesis reactor. Simple GA has the tendency to locate the near global optima but not necessarily the global optima [7]. Also, Upreti & Deb [31] have not tried all possible combinations of key parameters (p_c - crossover probability, p_m - mutation probability, N - population size). Moreover, there is a contradiction in the temperatures & gas flow rate profiles obtained. They reported the profiles that were not so smooth as in earlier literature. Also, they reported reverse reaction condition at the top temperature of 664 K which was not found in literature earlier. Hence, the present study is carried out in order to take care of the above deficiencies.

Differential Evolution (DE) is an improved version of simple GA. It is exceptionally simple, significantly faster & robust at numerical optimization and is more likely to find a function's true global optimum [2, 3, 5, 9, 10, 11, 26, 35]. DE has been

successfully applied in various fields. The various applications of DE include: digital filter design [30], fuzzy decision making problems of fuel ethanol production [33], Design of fuzzy logic controller [27], batch fermentation process [12, 32], multi sensor fusion [18], dynamic optimization of continuous polymer reactor [20], estimation of heat transfer parameters in trickle bed reactor [9], optimal design of heat exchangers [6, 7], synthesis & optimization of heat integrated distillation system [8], optimization of non-linear functions [2], optimization of an alkylation reaction [4], scenario- integrated optimization of dynamic systems [5], optimization of thermal cracking operation [3], optimization of non-linear chemical processes [10], global optimization of MINLP problems [11], determining the number of components in mixtures of linear models [13], Identification of hysteretic systems using the differential evolution algorithm [19], optimization of Low Pressure Chemical Vapour Deposition Reactors Using Hybrid Differential Evolution [21], hybrid differential evolution for problems of Kinetic Parameter Estimation and Dynamic Optimization of an Ethanol Fermentation Process [34] etc.

This paper presents the effective use of DE to optimize the system's objective function subject to a number of equality constraints involving solution of coupled differential equations. The three-coupled differential equations are solved using two different techniques (to check if it was the limitation of numerical methods because of which reverse reaction trend was not reported earlier), namely, Runge-Kutta method with variable step size, and Gear's method [17]. This paper also introduces the concept of "Nested DE" technique wherein the outer DE optimizes the optimization parameters (CR, F, NP) of inner DE.

2. PROBLEM FORMULATION

The Problem formulation is similar to that given in [22] including the modifications mentioned in [31]. Feed gas contains 21.75 mole% nitrogen, 65.25 mole% hydrogen, 5 mole% ammonia, 4 mole% methane and 4 mole% argon. In a typical ammonia synthesis reactor, feed gas enters the reactor from the bottom. The yield of ammonia depends on the temperature of feed gas at the top of the reactor (henceforth called top temperature), the partial pressures of the reactants (nitrogen and hydrogen), and the reactor length. As shown in [31], the final corrected objective function is:

$$F = 1.33563 \times 10^7 - 1.70843 \times 10^4 N_{N_2} + 704.09(T_g - T_0) - 699.27(T_f - T_0) - [3.45663 \times 10^7 + 1.98865 \times 10^9 x]^{0.5} \quad (1)$$

It is clear from the above expression that the objective function depends on four variables: the reactor length x , proportion of nitrogen N_{N_2} , the reacting gas temperature T_g , and the feed gas temperature T_f , for a given top temperature T_0 . From the system model, we have three differential equations and four variables, making the degrees of freedom equal to one. We specify the length of the reactor, calculate the remaining

variables using the system model and then pass these variables to the optimization routine. The computation procedure for the optimization carried out is shown in Fig. 1.

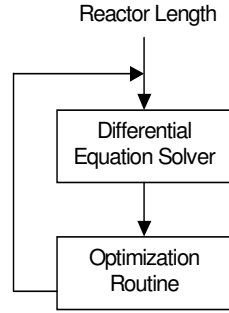
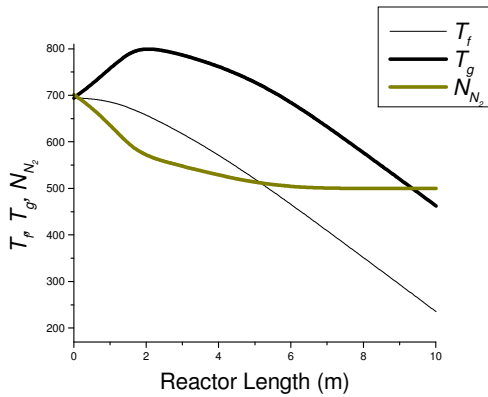


Fig 1. Computation Procedure

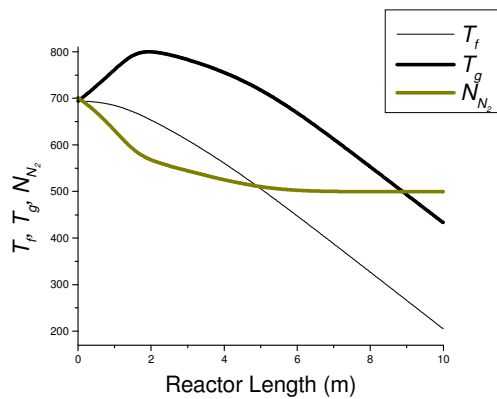
3. RESULTS & DISCUSSION

3.1. Temperature & Flow rate Profiles

First, the system equations were solved using Runge-Kutta variable step size method (RKVS). It is evident from the graph that the profiles are smooth and there are no spikes as reported in [31]. Therefore, in order to check if it is the limitation of RKVS method because of which spikes are not obtained, the other numerical method viz. Gear's method (GEAR) is also used for simulating the results.



(a) RKVS



(b) GEAR

Fig 2. The Profiles obtained using two Numerical Methods

Figs. 2 (a) & (b), show the profiles obtained using the above two methods. The profiles obtained are quite smooth, without any spikes and are similar to those obtained with RKVS. The profiles are same qualitatively but they differ slightly quantitatively. To illustrate the exact difference quantitatively, the above observations & comparison of various numerical methods used for simulating the results are presented in Table-1 for the reactor lengths of 10 m. Table-2 & Table-3 show the reactor length for which the variables N_{N_2} & T_g and N_{N_2} & T_f intersect respectively. From the Table-1, Table-2 and Table-3, it is evident that the two numerical methods (stated above) are equally good barring a few of the following differences. The difference in prediction of intersections is less than 5.0% between RKVS & GEAR method. RKVS is latest & has the ability to adopt its step size and varies as per requirement at every move. Based on the above observations, it can be substantiated that all the six methods are equally good both qualitatively giving the same results and quantitatively with slight difference. Hence, any one of the above numerical methods can be used for the solution of three coupled differential equations.

Table-1. Comparison of different Numerical Methods at a reactor length of 10 m.

Methods Parameters	RKVS	GEAR
x	10.00	10.00
N_{N_2}	499.68	499.46
T_g	462.86	432.69
T_f	235.71	204.73

Table-2. Reactor Length at which variables N_{N_2} & T_g intersect

Methods Parameters	RKVS	GEAR
x	9.355	8.895
N_{N_2}, T_g	499.68	499.57

Table-3. Reactor Length at which variables N_{N_2} & T_f intersect

Methods Parameters	RKVS	GEAR
x	5.156	4.900
N_{N_2}, T_f	511.75	511.55

Upreti & Deb [31] reported that the reverse reaction predominates the forward reaction at the top temperature of 664 K. In the present study, the two methods quoted above were used to generate temperature & flow rate profiles at that temperature. Surprisingly, there is no such trend observed in the profiles obtained [for which Upreti & Deb [31] gave a very good physical explanation] as can be seen in Fig 3 plotted using the results obtained with RKVS. To see the presence of any reverse reaction effect, the program is executed for temperatures even below 664 K with interval of 10 K up to 600 K. But no such trend is observed even at a top temperature as low as 600 K. Also, Upreti & Deb [31] reported that the three differential equations become unstable at the top temperature of 706 K.

However, using the above stated numerical methods, it is observed that the equations are not unstable even at a top temperature as high as 800 K. It may be noted that Upreti & Deb [31] used NAG library's subroutine D02EBF (which is now replaced by D02EJF [23]). So it may be because of the problem in the software package that they reported the reversible reaction effect.

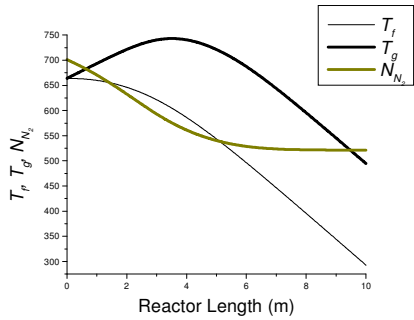
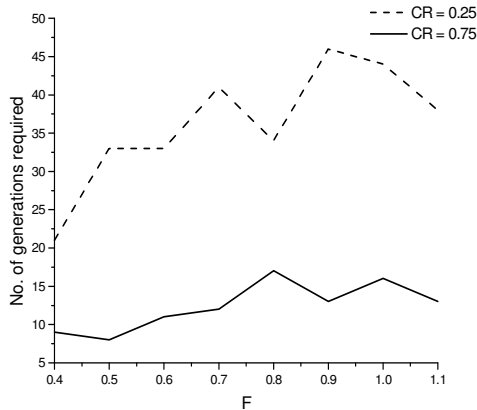
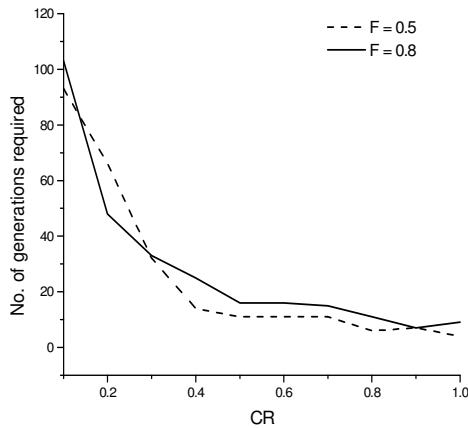


Fig 3. The profiles obtained using RKVS



(a) Constant CR



(b) Constant F

Fig 4. The Effect of F and CR on Number of generations

3.2. Optimization of reactor length using DE

Price & Storn [24] gave the working principle of DE with single strategy. Later on, they suggested ten different strategies of DE [25]. DE is an improved version of GA for faster optimization. Among the DE's advantages are its simple structure, ease of use, speed and robustness. The advantages of DE over its similar counterparts such as simple GA, simulated annealing are evident from the results presented in [2, 11]. The key parameters of control are: NP - the population size, CR - the crossover constant, F - the weight applied to random differential (scaling factor).

3.2.1. Selection of parameters for DE: Choosing NP, F, and CR depends on the specific problem applied, and is often difficult. But some general guidelines are available. Normally, NP should be about 5 to 10 times the number of parameters in a vector. As for F, it lies in the range 0.4 to 1.0. Initially F = 0.5 can be tried then F and/or NP is increased if the population converges prematurely. A good first choice for CR is 0.1, but in general CR should be as large as possible [24]. The best combination of these key parameters of DE for each of the strategies mentioned earlier is again different. Price & Storn [25] have mentioned some simple rules for choosing the best strategy as well as the ranges of corresponding key parameters.

The key parameters are generally found by trial & error method. In this method one parameter is kept constant while varying the others in steps. In this process we may miss out optimum combination that gives global optima, as it is very difficult to cover the entire range of all the key parameters, however small the incremental step may be. The comparison of results obtained using different combination of DE key parameters (CR and F) are shown in Fig. 4 (a) and (b). These graphs show us how difficult it is to find out which combination can be the most suitable one for our problem as there is no specific trend observed.

3.3. "Nested DE" – A new Concept

By looking at the problems mentioned above and the results obtained in the present study in choosing the right combination of the DE key parameters, it was felt that DE itself could be used for finding the optimum key parameters along with the optimum variables of the actual problem formulation (i.e. using DE within DE wherein outer loop takes care of optimization of key parameters (NP, CR, F) of inner DE with the objective of minimizing the number of generations required (G_{min}), while inner loop taking care of optimizing the problem variables). Yet complex objective can be the one that takes care of minimizing the number of generations/function evaluations & the standard deviation (SD) in the set of solutions at the last generation/function evaluation, and try to maximize the robustness of the algorithm. Initially, the tuning parameters for outer DE (NP_OUTER, CR_OUTER & F_OUTER) were chosen on the basis of general heuristics (Section 3.2.1). The effect of varying these tuning parameters of the outer DE is discussed in detail later in this section. The optimum reactor length obtained using GEAR with "Nested DE" is 6.79 m (at top temperature of 694) with objective function value of \$4848383.0 per year. The difference in the optimum reactor length found using two methods can be attributed to the small quantitative differences in the simulated profiles as explained in Section 3.1. To find the best combination of these parameters for the present problem, we varied CR & F, but kept NP to the higher side (NP=10*D, for being on the safer side). The algorithm followed for the "Nested DE" operation in combination with GEAR is shown in Fig. 5.

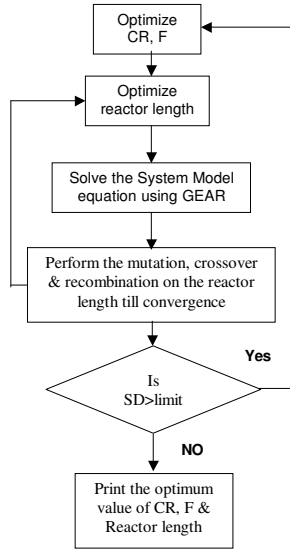


Fig 5. The Solution Strategy For “Nested DE”

The optimum DE parameters using “Nested DE” (with the strategy DE/rand/1/bin) with GEAR method for various standard deviations are shown in Table-4. For population of x_i 's ($i=1,2,3\dots NP$), we define

$$\text{Standard Deviation (SD)} = \sqrt{\frac{\sum_{i=1}^{NP} (\bar{x} - x_i)^2}{NP - 1}} \quad (2)$$

$$\text{Where, } \bar{x} = \frac{\sum_{i=1}^{NP} x_i}{NP} \quad (3)$$

The pseudo code for ‘Nested DE’ used in the present study is given below:

1. Choose the DE strategy to be used for both the inner and the outer DE.
2. Initialize the variable D for both inner ($D_INNER = 1$, the reactor length (x)) and outer ($D_OUTER=2$, CR_INNER & F_INNER for inner DE) DEs
3. Initialize the tuning parameters NP_OUTER , CR_OUTER & F_OUTER for the outer DE.
4. Initialize the initial population of NP_OUTER (DE) points within the defined limits for the variables CR_INNER & F_INNER as follows:

```

for(iouter = 1; iouter <= NP_OUTER; iouter++)
{
  innerCR[iouter] = CR_INNER_LOWER_LIMIT +
  Random_Number *
  (CR_INNER_LOWER_LIMIT -
  CR_INNER_LOWER_LIMIT);
  innerF[iouter] = F_INNER_LOWER_LIMIT +
  Random_Number * (F_INNER_LOWER_LIMIT
  - F_INNER_LOWER_LIMIT);
}
  
```

5. Calculate the number of generations required for the inner DE to converge to the global optima using the recent population of $innerCR[i]$ & $innerF[i]$ tuning parameters for all NP_OUTER points of the recent generation.

```

for(iouter = 1; iouter <= NP_OUTER; iouter++)
{
  Generations_Required[iouter] =
  innerDE(innerCR[iouter], innerF[iouter]);
}
  
```

- 5a. Initialize the initial population for the inner DE:

```

for(iinner = 1; iinner <= NP_INNER; iinner++)
{
  x[iinner] = X_LOWER_LIMIT +
  
```

```

  Random_Number*(X_LOWER_LIMIT -
  X_LOWER_LIMIT);
}
  
```

- 5b. Calculate the value of profit function for all x 's by performing simulation using the chosen differential equation solver (eg. RKVS, and GEAR, etc.).

```

for(iinner = 1; iinner <= NP_INNER; iinner++)
{
  [Ti[iinner], Tg[iinner], NN2[iinner]] =
  simulate_profiles(x[iinner]);
  Profit[iinner] = profit_function(x[iinner],
  Ti[iinner], Tg[iinner], NN2[iinner]);
}
  
```

- 5c. Form the next generation for inner DE by performing mutation, recombination and selection (specific to the chosen DE strategy) with the tuning parameters $innerCR[iinner]$ and $innerF[iinner]$. For the present study, the seventh DE strategy (DE/rand/1/bin) was used. The steps involved are randomly choosing 3 vectors (a , b , c ; distinct from the target vector i) against which the trial vector will be checked) from the NP_INNER vectors of the present generation and then continuing as follows:

```

Let i be the index of the target vector.
x_trial = x[a] + innerF[iouter]*(x[b]-x[c]);
[Ti_trial, Tg_trial, NN2_trial] =
simulate_profiles(x_trial);
Profit_trial = profit_function(x_trial, Ti_trial,
Tg_trial, NN2_trial);
if( Profit[i] < Profit_trial )
  pass the trial vector into the next generation
  to replace the target vector
else
  retain the target vector for the next
  generation
  
```

- 5d. Check if the standard deviation (using Eqs. 17 & 18) for the present generation has gone below the maximum allowable limit (SD). If this condition is met, go to the next step, else, go to step 5b.

- 5e. Report the number of generations required for inner DE to reach the SD to the outer DE.

6. Form the next generation for outer DE by performing mutation, recombination and selection (specific to the chosen DE strategy) with the tuning parameters CR_OUTER and F_OUTER . As explained in step 5c, this was done using the seventh DE strategy. Similar calculations will follow.

```

Let i be the index of the target vector.
innerCR_trial = (Random_Number < CR_OUTER ?
  (innerCR[a] + F_OUTER*(innerCR[b]-
  innerCR[c])): innerCR[i]);
innerF_trial = (Random_Number < CR_OUTER ?
  (innerF[a] + F_OUTER*(innerF[b]-innerF[c])):
  innerF[i]);
Generations_Required_trial = innerDE(innerCR_trial,
innerF_trial);
if( Generations_Required[i] <
Generations_Required_trial )
  pass the trial vector into the next generation to
  replace the target vector
else
  retain the target vector for the next generation
  
```

7. Check the termination criteria (Either reaching the maximum number of generations allowed or reaching the standard deviation below SD) for outer DE is satisfied. If yes, go to next step, else, go to step 5.

8. Print the results.

Table-4. Optimum DE parameters Using “Nested DE” with GEAR for various SD values

SD	Reactor Length (m)	Objective Function (10 ⁶ \$/year)	CR	F	G _{min}
1.0	6.79	4.848	0.745	0.520	1
0.5	6.79	4.848	0.939	0.485	2
0.25	6.79	4.848	0.995	0.701	4
0.1	6.79	4.848	0.868	0.553	6
0.01	6.79	4.848	0.902	0.434	10
0.001	6.79	4.848	0.793	0.437	18

From Table-4, it is clear that irrespective of the values of SD (1.0, 0.5, 0.25, 0.1, 0.01 & 0.001) and the corresponding CR & F values, we obtained almost same values of the objective function (4848383.0 \$/year) and reactor length (6.79 m). It consolidates the robustness of the DE algorithm. The more wider the range of values of CR, F, and SD for which same values of objective function and reactor length are obtained, the more robust is the algorithm. Also, the code of “Nested DE” was run with another strategy DE/rand/1/exp, and found that results are exactly the same. Irrespective of the parameters used for outer DE, it was found that optimum key parameters (CR & F) of inner DE were almost same as shown in Table-5. This also proves DE’s power and robustness. Now that we have already tried the effect of DE parameters and strategy on speed and accuracy and found that it has little or no effect on accuracy, we can say that the NP in a generation, if taken within the limits, would not have any effect on the result.

Table-5. Optimum Key Parameters of inner DE with different combinations of CR & F for outer DE

S. No.	CR OUTER	F OUTER	Optimum Reactor Length (m)	Profit Function (10 ⁶ \$/year)	Optimum inner CR	Optimum inner F	G _{min}
1	0.4	0.8	6.790	4.85	0.931	0.431	16
2	0.5	0.8	6.790	4.85	0.921	0.452	16
3	0.6	0.8	6.790	4.85	0.954	0.442	17
4	0.7	0.8	6.790	4.85	0.960	0.433	16
5	0.8	0.8	6.790	4.85	0.924	0.425	16
6	0.9	0.8	6.790	4.85	0.947	0.433	15
7	0.9	0.5	6.790	4.85	0.956	0.452	16
8	0.9	0.6	6.790	4.85	0.938	0.444	16
9	0.9	0.7	6.790	4.85	0.937	0.456	16
10	0.9	0.8	6.790	4.85	0.920	0.449	16
11	0.9	0.9	6.790	4.85	0.934	0.432	16

Table-6 shows the results obtained from different methods & its comparison with those obtained in [22, 15, 31] using Pontryagin’s maximum principle (PMP), Lasdon’s generalized reduced-gradient method (LGRG) & Genetic Algorithm (GA) respectively. From Table-6, we observe that an optimum reactor length of 2.58 m is reported in [15] and 5.18 m in [22], both of which are wrong due to the errors in their problem formulations as pointed out in [31]. An optimum reactor length of 5.33 m and the corresponding objective function value is 4.23x10⁶ \$/year, reported in [31] are also not correct as found in the present study. Among other methods, GEAR & RKVS have the same objective function value though the optimum reactor length is slightly different in each case. Also, the present study establishes the accuracy and robustness of DE. Hence, the correct optimum reactor length can be considered as 6.79 m with an objective function value of 4.84x10⁶ \$/year.

Table-6. Optimum Reactor Length & Objective function using various Numerical Methods

Methods Parameters	PMP [22]	LGRG [15]	D02EBF With GA [31]	GEAR With DE	RKVS With DE
Optimum X (m)	5.18	2.58	5.33	6.79	7.16
Objective function (10 ⁶ \$/year)	Not Reported	1.29	4.23	4.84	4.84

4. CONCLUSIONS

In the present study Differential Evolution (DE) is used for the optimal design of an auto-thermal ammonia synthesis reactor. The new concept of “Nested DE” is introduced wherein the speed and convergence of the inner DE loop optimizing the system’s objective function are controlled by the outer DE loop, which optimizes the inner DE’s tuning parameters. Results indicate that the profiles of temperatures & flow rate are smooth and there is no reverse reaction effect irrespective of numerical method used for the solution of differential equations. The optimum reactor length depends upon the top temperature. Also, the power & robustness of DE is brought out using new concept of “Nested DE”. At the top temperature of 694 K, the reactor length of 6.79 m was found to give the optimum objective function value of \$ 4.84x10⁶/year. This successful application of DE for the optimal design of ammonia synthesis reactor indicates that DE has great potential and can be applied to advantage in all the highly non-linear & complex engineering problems.

5. REFERENCES

- [1] D. Annable, “Application of the Temkin Kinetic Equation to Ammonia Synthesis in Large – Scale Reactors”, **Chemical Engineering Science**, 1(4), 145, 1952.
- [2] B. V. Babu & Rakesh Angira, “Optimization of Non-linear Functions using Evolutionary Computation”, **Proceedings of 12th ISME Conference**, Chennai, India, Jan, 10–12, 153-157, 2001. Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#34>
- [3] B. V. Babu & Rakesh Angira, “Optimization of Thermal Cracker Operation using Differential Evolution”, **Proceedings of 54th Annual Session of IChE**, CLRI, Chennai, December 19-22, 2001. Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#38> & Application No. 20, Homepage of Differential Evolution, the URL of which is: <http://www.icsi.berkeley.edu/~storn/code.html>
- [4] B. V. Babu & C. Gaurav, “Evolutionary Computation Strategy for Optimization of an Alkylation Reaction”, **Proceedings of 53rd Annual Session of IChE**, Calcutta, December 18-21, 2000. Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#31>
- [5] B. V. Babu & K. Gautam, “Evolutionary Computation for the Scenario-Integrated Optimization of Dynamic Systems”, **Proceedings of 54th Annual Session of IChE**, CLRI, Chennai, December 19-22, 2001. Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#39>

- [6] B. V. Babu & S. A. Munawar, "Differential Evolution for the Optimal Design of Heat Exchangers", **Proceedings of All-India seminar on Chemical Engineering Progress on Resource Development: A Vision 2010 and Beyond**, IE (I), Bhubaneswar, India, March 11, 2000. Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#35>
- [7] B. V. Babu & S. A. Munawar, "Optimal Design of Shell & Tube Heat Exchanger by Different strategies of Differential Evolution", **PreJournal.com - The Faculty Lounge**, Article No. 003873, posted on website <http://www.prejournal.com>, March 03 (2001). Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#28>
- [8] B. V. Babu & Rishinder Pal Singh, "Synthesis & Optimization of Heat Integrated Distillation Systems Using Differential Evolution", **Proceedings of All-India seminar on Chemical Engineering Progress on Resource Development: A Vision 2010 and Beyond**, IE (I), Bhubaneswar, India, March 11, 2000.
- [9] B. V. Babu & K. K. N. Sastry, "Estimation of Heat-Transfer Parameters in a Trickle-Bed Reactor using Differential Evolution and Orthogonal Collocation", **Computers & Chemical Engineering**, 23, 327-339, 1999. Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#24>
- [10] B.V. Babu & Rakesh Angira, "Optimization of Non-Linear Chemical Processes Using Evolutionary Algorithm", **Proceedings of International Symposium & 55th Annual Session of IChE**, OU, Hyderabad, December 19-22, 2002. Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#53>
- [11] B.V. Babu & Rakesh Angira, "A Differential Evolution Approach for Global Optimization of MINLP Problems", **Proceedings of 4th Asia-Pacific Conference on Simulated Evolution And Learning**, Singapore, November 18-22, 2002. Also available via Internet as .pdf file at <http://bvbabu.50megs.com/custom.html/#45>
- [12] J. P. Chiou & F. S. Wang, "Hybrid Method of Evolutionary Algorithms for Static and Dynamic Optimization Problems with Application to a Fed-batch Fermentation Process", **Computers & Chemical Engineering**, 23, 1277-1291, 1999.
- [13] S. Dollena Hawkins, M. Allen David and J. Stromberg Arnold, "Determining the Number of Components in Mixtures of Linear Models. **Computational Statistics & Data Analysis**, 38, 15-48, 2001.
- [14] D. C. Dyson, **Optimal Design of Reactors for Single Exothermic Reversible Reactions**, Ph.D. Thesis, London University, 1965.
- [15] T. F. Edgar & D. M. Himmelblau, **Optimization of Chemical Processes**. Singapore, McGraw-Hill, Inc., Page Nos. 534-539, 1989.
- [16] J. Eymery, **Dynamic Behavior of an Ammonia Synthesis Reactor**, D. Sc. Thesis, M.I.T., 1964.
- [17] S. K. Gupta, **Numerical Methods for Engineers**. Wiley Eastern Limited, Delhi (India), 1995
- [18] R. Joshi & A. C. Sanderson, "Minimal Representation Multi-Sensor Fusion using Differential Evolution", **IEEE Transactions on Systems, Man and Cybernetics, Part A** 29, 63-76, 1999.
- [19] A. Kyprianou, K. Worden, and M. Panet, "Identification of Hysteretic Systems using the Differential Evolution Algorithm", **Journal of Sound and Vibration**, 248 (2), 289-314, 2001.
- [20] M. H. Lee, C. Han, and K. S. Cheng, "Dynamic Optimization of a Continuous Polymer Reactor using a Modified Differential Evolution", **Industrial & Engineering Chemistry Research**, 38(12), 4825-4831, 1999.
- [21] J. C. Lu & F. S. Wang, "Optimization of Low Pressure Chemical Vapour Deposition Reactors Using Hybrid Differential Evolution", **Canadian Journal of Chemical Engineering**, 79 (2), 246-254, 2001.
- [22] A. Murase, H. L. Roberts, and A. O. Converse, "Optimal Thermal Design of an Autothermal Ammonia Synthesis Reactor", **Industrial & Engineering Chemistry Research**, 9, 503- 513, 1970.
- [23] *Web site of Numerical Algorithm Group* as on March, 2004. http://www.nag.com/numeric/FL/manual/html/genint/FL_withdrawn.asp
- [24] K. Price & R. Storn, "Differential Evolution – A Simple Evolution Strategy for Fast Optimization", **Dr. Dobbs's Journal**, 22 (4), 18-24 & 78, 1997.
- [25] K. Price & R. Storn, *Home Page of Differential Evolution* as on March, 2004. <http://www.ICSI.Berkeley.edu/~storn/code.html>.
- [26] Günter Rudolph, "Convergence of Evolutionary Algorithms in General Search Spaces", **Proceedings of the 3rd IEEE International Conference on Evolutionary Computation**, 20-22 May 1996, Nagoya, Japan, pp.50-54. ISBN 0-7803-29023.
- [27] K. K. N. Sastry, L. Behra, and I. J. Nagrath, "Differential Evolution based Fuzzy Logic Controller for Nonlinear Process Control", **Fundamenta Informaticae: Special Issue on Soft Computation**, 1998.
- [28] M.J.Shah, "Control Simulation in Ammonia Production", **Industrial & Engineering Chemistry**, 59, 72, 1967.
- [29] C. P. P. Singh, & D. N. Saraf, "Simulation of Ammonia Synthesis Reactors", **Industrial & Engineering Chemistry Process Design Development**, 18(3), 364-370, 1979.
- [30] R. Storn, "Differential Evolution Design of an IIR-filter with Requirements for Magnitude and Group Delay", TR-95-018, International Computer Science Institute, 1995.
- [31] S. R. Upreti, & K. Deb, "Optimal Design of an Ammonia Synthesis Reactor using Genetic Algorithms", **Computers & Chemical Engineering**, 21, 87– 92, 1997.
- [32] F. S. Wang & W. M. Cheng, "Simultaneous Optimization of Feeding Rate and Operation Parameters for Fed-batch Fermentation Processes", **Biotechnology Progress**, 15(5), 949-952, 1999.
- [33] F. S. Wang, C. H. Jing, and G. T. Tsao, "Fuzzy-Decision-Making Problems of Fuel Ethanol Production using Genetically Engineered Yeast", **Industrial & Engineering Chemistry Research**, 37, 3434-3443, 1998.
- [34] F. S. Wang, T. L. Su, and H. J. Jang, "Hybrid Differential Evolution for Problems of Kinetic Parameter Estimation and Dynamic Optimization of an Ethanol Fermentation Process", **Industrial & Engineering Chemistry Research**, 40 (13), 2876-2885, 2001.
- [35] Daniela Zaharie, "Critical Values for Control Parameters of Differential Evolution Algorithms", In Radek Matoušek and Pavel Ošmera (eds.) (2002). **Proceedings of MENDEL 2002, 8th International Conference on Soft Computing**, June 5-7, 2002, Brno, Czech Republic. Brno University of Technology, Faculty of Mechanical Engineering, Institute of Automation and Computer Science, Brno (Czech Republic), pp.62-67. ISBN 80-214-2135-5.