EVOLUTIONARY COMPUTATION FOR SCENARIO- INTEGRATED OPTIMIZATION OF DYNAMIC SYSTEMS

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Abstract: In any Chemical Process Industry, it is necessary to assess the consequences of unexpected events such as equipment failures, change of raw material prices and product demand. In this work, these unexpected events are called "scenarios", which allow the determination of operational strategies that are economically optimal and keep the plant within a chosen regime in the state space. This is achieved by the consideration of several scenarios. The formulations in this paper are based on a unifying model framework containing both discrete and continuous dynamics. Taking the case of a single scenario, Differential Evolution is used for the scenario- integrated dynamic optimization of the formulated problem. The applicability of this technique is demonstrated with an example.

Key Words: Scenario-Integrated Optimization, Dynamic Systems, Evolutionary Computation, Differential Evolution, DE Strategies.

INTRODUCTION

In any chemical process plant, there are several process units that are present. In order to simulate their functioning, it is essential to model these units as accurately as possible. Dynamic modeling is used when the system under consideration is a dynamic one or one that is presently operating under an unsteady state. The commonest examples of such cases where dynamic simulation becomes a necessity are batch and semibatch reactors. In fact, all continuous processes require dynamic simulation during startup and shutdown.

Presently, the focus of the process industry has been not only on determining the conventional mode of operation of a system but on finding the optimal mode, or at least, an improved mode of operation. The normal practice is to apply a large number of input functions and to formulate the problem as one of the dynamic simulation type. Conventional numerical techniques are applied to solve such problems. The attempt of this work has been to apply the relatively new "Differential Evolution" technique to the same problems. The effect of uncertainties on the behavior of the system has to be investigated. These situations may arise from unexpected changes in the environment or from changes in the system itself. Examples of these situations are changing market prices and unexpected equipment failures. In this paper, such a hypothetical situation initiated at a specific time is called a *scenario* [Abel et al., 2000]. The question that arises is that whether the treatment of scenarios and the optimization of dynamic systems could be clubbed together to give an integrated design procedure. The resultant procedure that arises by combining the two techniques mentioned to give an integrated design procedure is called *robust optimization.* In most problems, there are uncertain parameters present. These uncertain parameters are assumed to be constant in certain cases. But this assumption is not always justified.

When certain parts of the problem cannot be expressed deterministically, optimization must be carried out with the help of probabilities attached to certain parameters. Such an attempt is called *stochastic optimization.* Usually, a probability density function of all the unknown parameters is known [Birge and Louveaux, 1997]. This probability density function is usually assumed to be constant over the time period under consideration. If the probability function changes with time, it would become necessary to descretize the probability function in terms of time intervals. In other words, to deal with the complexity of the situation, we discretize one of the problem co-ordinates. In the treatment of such problems of dynamic simulation the observation of parameter values becomes imperative. This leads to the formation of a *scenario tree* of possible parameter values over time. Some of the motivating examples of problems that need dynamic simulation are discussed below.

EXAMPLES OF DYNAMIC SIMULATION PROBLEMS

As mentioned above, optimization under uncertainty is called *stochastic optimization*. This approach is an

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attempt to find the optimal decision variables when certain parts of the problem formulation cannot be described deterministically. An obvious extension of this type of problem is to allow parameter changes at arbitrary instants over a period of time of interest. A third level of complexity arises because the number of possible time instants is infinite. This situation is dealt with by discretizing one of the co- ordinates. When the problem is formulated in discrete time, the instants under consideration are called *stages.* The resulting formulations are called multi- stage stochastic programming problems.

Example 1: Batch- Distillation Column. Batch-Distillation columns are often operated at temperatures that are significantly different from the ambient temperature. Since the heat exchange with the environment depends on the existing temperature difference, the quality of the distillate can suffer from sudden changes in the ambient conditions if the time varying operational strategy is not appropriately adopted. For example, such a sudden change in the ambient conditions results from cold rain on a hot day. Again it may be unknown if the weather conditions will indeed change. If they change, the instant at which rain will start, as well as the associated temperature decreases are unknown. These problems are always of combinatorial complexity. For only a single uncertain parameter with n samples of parameter values and k stages over time, the number of possible scenarios are already n^k. The economic objective used has now to be evaluated for all the n^k number of scenarios distinguished by n^k different parameter values. For the optimal operation of a chemical process under uncertainty, the approaches used have to cope with changes that not only influence certain parameters but that also affect the structure of the process. This is illustrated by the example below.

Example 2: Semibatch reactor with partial cooling-system failure. In the operation of highly exothermic semibatch reactors, multiple cooling systems are sometimes used. One part of the cooling system often consists of a jacket surrounding the reactor, and a second part is provided by a coil in the vessel. If one of the cooling systems fail during a batch, the feed flow rate to the reactor and the cooling strategy of the remaining system must be changed in order to ensure the feasibility of the existing constraints and to ultimately save the batch to the extent possible. Another example of similar nature is that of a *Two- Phase semibatch reactor with stirrer failure.* In this case, when the stirrer fails, areas with slower reaction rates can be distinguished from areas with faster reaction rates. However, a batch might still be operated to the endpoint if the trajectories of the feed flow rate and the desired temperature are adapted appropriately. The problems discussed so far fall into one of the two sub- classes of optimization problems. These are called *single level scenario- integrated optimization problems.* In this class of problems, the nature of the scenarios and the operational goals favor the use of a single economic objective function independently of any change or event that might happen during the transient process. The second class of problems are the *bilevel (or multi level) scenario- integrated optimization problems.* The following example illustrates the above group.

Example 3. Semibatch reactor, reconsidered. Sometimes, emergency rules might suggest that the process be shut down after the loss of the cooling system, preventing any further economic optimization. The time to reach operating conditions characterized by low temperatures and pressures might then be used as the secondary goal for the time after the failure.

SCENARIO- INTEGRATED MODELING

The phenomena initiating a scenario usually occurs on a much shorter time scale than the nominal dynamics of the chemical processes considered. We therefore assume that these changes can be described by an instantaneous event. The resulting discrete elements render the scenario integrated model description of a hybrid (discrete-continuous) nature [Alur et al., 1995; Barton and Pantelides, 1994]. For the proper definition of a hybrid system, three issues have to be tackled; the continuous part, the discrete part and the interaction between the two [Abel et al., 2000]. This article deals only with a single transition system. The theory of hybrid systems provides a convenient basis for the development of scenario- integrated models for dynamic systems [Abel et al., 2000].

SCENARIO- INTEGRATED OPTIMIZATION

Having considered model formulations for dynamic systems with incorporated scenarios, we can now start to consider their dynamic optimization. Unfortunately, the theory of hybrid systems does not provide an equally sound basis as for modeling and simulation. This is because the number and the type of transitions can change during the search for a set of optimum profiles. But the case under consideration is one of a single transition. This is a relatively simple case and can be dealt with. This class of problems is called *Single level Scenario- Integrated Optimization Probems.* If the number of possible scenario modes is restricted to one and if the switching time is assumed to be known, the existing uncertainty is reduced to the question of whether or not the event triggering the scenario will occur. This situation is illustrated by Figure 2. The system evolves in the nominal mode along the trajectories of $u_o(t_0)$ and $x_0(t_0)$ upto the switching time $t^*_{0,1}$. Then it may switch to the scenario mode ξ=0. The optimization problem is to find profiles of the available operational degrees of freedom $u_o(t_0)$ and $u_1(t_1)$, which will minimize the chosen objective function under the set of given constraints.

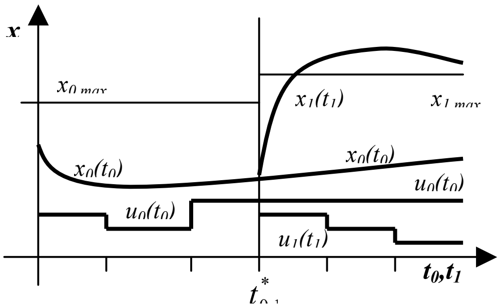


Figure 2. Evolution of a state and manipulated variable within the nominal and scenario mode.

For a single-level problem, if the constraints are denoted by g_0 and g_1, the model proposed by Abel et al., 2000 is given below. This model is called the SIOP1 model or the Scenario- Integrated Optimization Problem 1 model.

$$\min_{\substack{x_{0,0},u_0(t_0),t_{0,f},\\ u_1(t_1),t_{1,f}}} w_0\Phi_0(x_0,y_0,u_0,t_{0,f})+w_1\Phi_1(x_1,y_1,u_1,t_{1,f})$$

$$\begin{aligned} s.t.\ 0 &= f_0(\dot{x}_0,x_0,y_0,u_0,t_0) \\ 0 &= x_0(t_{0,0})-x_{0,0} \\ 0 &\geq g_0(x_0,y_0,u_0,t_0) \quad \forall t_0 \in \left[t_{0,0},t_{0,f}\right] \\ 0 &= f_1(\dot{x}_1,x_1,y_1,u_1,t_1) \\ 0 &= h_{0,1}(x_0,u_0,x_1,u_1,t^*_{0,1}) \\ 0 &\geq g_1(x_1,y_1,u_1,t_1) \quad \forall t_1 \in \left[t^*_{0,1},t_{1,f}\right] \end{aligned}$$

(SIOP 1)

The initial conditions for the nominal mode $x_{0,0}$ and for the final times have been regarded as degrees of freedom. If these variables are fixed for specific problems, appropriate equations might be formulated as additional constraints.

DIFFERENTIAL EVOLUTION

Differential Evolution (DE) [Price and Storn, 1997) is a search procedure similar to Genetic Algorithms (GA) [Goldberg, 1989; Stair and Fraga, 1995; Upreti and Deb, 1996; Babu and Vivek, 1999; Babu and Mohiddin, 1999] applied on real world variables that is significantly fast at numerical optimization and is also more likely to find a function's true global optimum [Price and Storn, 1997]. Among DE's advantages are its simple structure, ease of use, speed and robustness. DE has been used for design and control applications [Chiou and Wang, 1999], estimation of heat transfer parameters in trickle bed reactor [Babu and Sastry, 1999], optimal design of heat exchangers [Babu and Munawar, 2000], optimal design of shell & tube heat exchanger [Babu and Munawar, 2001], synthesis & optimization of heat integrated distillation system [Babu and Rishinder Pal Singh, 2000], optimization of non-linear functions [Babu and Angira, 2001] etc. For the implementation of DE with a constrained problem, solutions were penalized on the fitness if any of the constraints were violated. The magnitude of the penalty was adjusted so as to significantly affect the fitness. Differential Evolution can be implemented in ten different strategies [Price and Storn, 2000].

In the present work, a comparative study of ten Differential Evolution strategies has been carried out when applied to Scenario Integrated Optimization of parameters in a semibatch reactor. A software routine DIFSOL is developed.

SCENARIO- INTEGRATED OPTIMIZATION FOR A SEMIBATCH REACTOR

The problem under study is that of a semibatch reactor as previously described in section 2. Let us say that strongly exothermic continuous reactions take place:

$$A \rightarrow B \rightarrow C$$

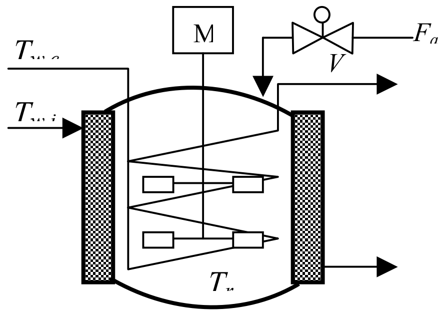


Figure 3. Semibatch Reactor.

The diagram of the reactor is shown in figure 3. Initially the vessel is supposed to be filled with a solvent. Then, component A is fed according to a specific recipe by adjusting valve V. While the temperature should follow a desired file, A reacts to B, which is partly consumed in order to form the undesirable component C. The vessel is equipped with two heat exchange systems, one through the reactor jacket (index *j*) and one using a coil inside the vessel (index *c*). Here the considered scenario is the possible failure of the jacket cooling system while the coil cooling system operates correctly. The kinetics are assumed to be first order and a single liquid phase is considered (Abel et al., 2000).

RESULTS AND DISCUSSION

Differential Evolution was utilized for the solving of the single level scenario- integrated optimization problem. The SIOP1 model (Abel et al., 2000) was used to define the problem of a semi- batch reactor with a partial cooling system failure. The Minimization problem was solved using all the ten strategies of Differential Evolution. In effect, the differential evolution program, DESOL, was run for different values of NP, F and CR. Figure 4 depicts the minima obtained for each strategy. It is evident that the 7th strategy of Differential Evolution is the optimal strategy because the minima obtained is the best. The subsequent graphs that are presented are for the 7th strategy of Differential Evolution, that is, DE/rand/1/bin. As discussed above, this involves the selection of only one set of random vectors and a binomial mode of selection for the reproduction operator.

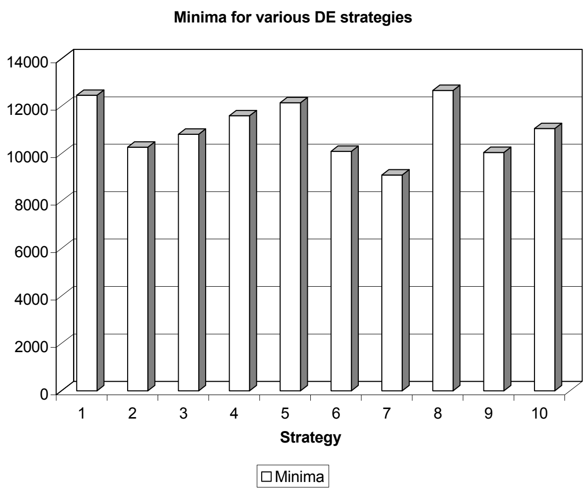


Figure 4. Minima for different strategies of Differential Evolution.

For the 7th strategy, Figures 5, 6 and 7 describe the variation of Standard Deviation vs the value of CR for different values of F and NP. The standard deviation calculated was about the minimum value for that value of F. The formula used for the computation of SD is (for $n = 10$):

$$SD = \sqrt{\sum_{i=1}^{9} \frac{(x_i - x_{\min})^2}{n-1}}$$

where, x_i is the min. for any CR value
x_{min} is the best min for that F
n = 10

As is evident from Figures 5, 6 and 7, there is no concrete trend between the variation between the values of SD for different values of F and CR.

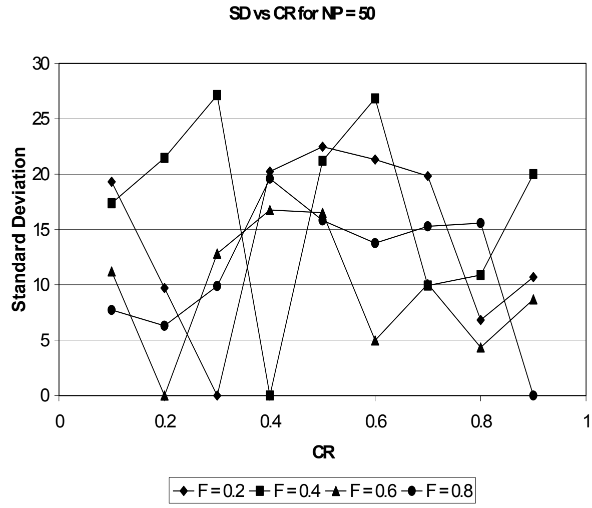


Figure 5. SD vs. CR for a Population size of 50.

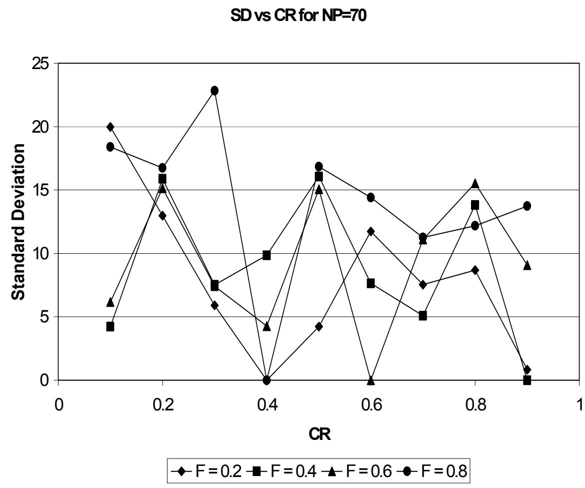


Figure 6. SD vs. CR for a Population size of 70.

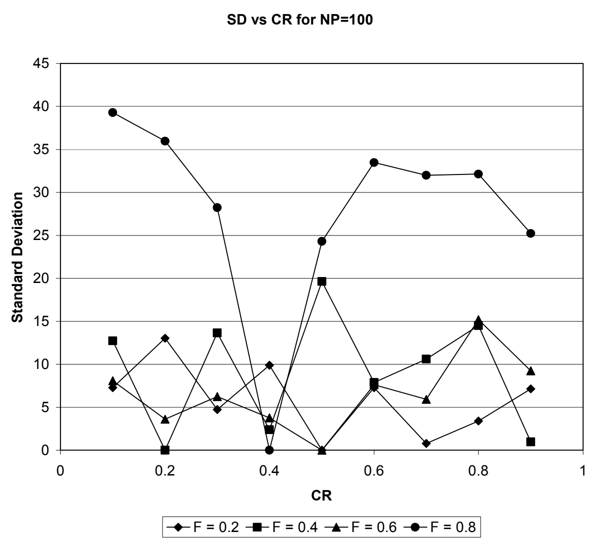
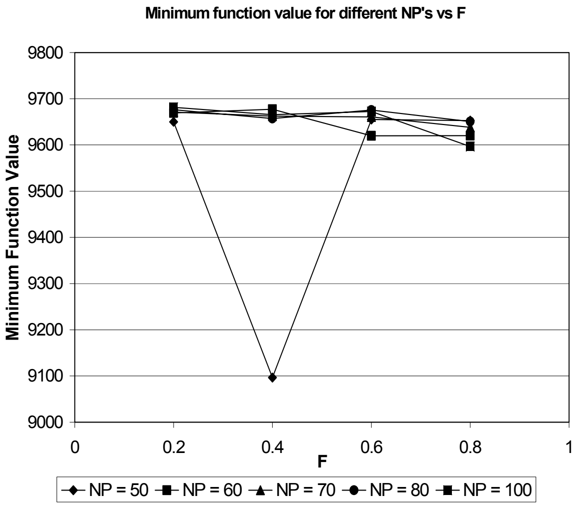


Figure 7. SD vs. CR for a population size of 100

From the figures 5, 6, and 7, it can be inferred that F = 0.4 is the most optimal for the 7th strategy of Differential Evolution when applied to the SIOP1 formulation. It can also be deduced that CR = 0.4 is the optimum value to be used for the above problem since the SD values at CR = 0.4 in Figures 5, 6 and 7 are zero for almost all values of F indicating that the best



minimum occurs at that point.

Figure 8. Minimum function value vs. F for various NP for DE/rand/1/exp.

Figure 8 indicates the different function values for different NP values against F. This graph shows a sharp dip for NP=50, CR=0.4, F=0.4 indicating that the global minimum has been attained.

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