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The Evolutionary Computation Techniques in Chemical Engineering

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ABSTRACT

Chemical process control requires intelligent monitoring due to the dynamic nature of the chemical reactions and the non-linear functional relationship between the input and output variables involved. Chemical reactors is one of the major processing unit in many chemical, pharmaceutical and petroleum industries as well as in environmental and waste management engineering. In spite of continuing advances in optimal solution techniques for optimization and control problems, many of such problems remain too complex to be solved by the known techniques.

The main aim of this thesis is to show that such a powerful optimizing tool like evolutionary algorithms (EAs) can be in reality used for the optimization and predictive control of chemical processes. Four algorithms from the field of artificial intelligent - Differential evolution (DE), Self-organizing migrating algorithm (SOMA), Genetic algorithm (GA) and Simulated annealing (SA) are used in this investigation. In the first section EAs were used to investigative and optimize of batch reactor to improve its parameters. Consequently, EAs are used to model the technical requirements for chemical reaction. The second section presents the optimizing of chemical engineering processes, particularly those in which the evolutionary algorithm is used for static optimization and control of Continuous stirred tank reactors (CSTRs).

The optimizations and control chemical reactors have been performed in several ways, each one for a different set of reactor parameters or different cost function. The optimized and predictive control chemical reactor processes were used in simulations with optimization by evolutionary algorithms and the results are presented in graphs. Finally, experimental results are reported, followed by conclusion.

Keywords: Optimization, Simulation, Evolutionary Algorithms, Batch, CSTR.

RESUMÉ

Vzhledem k dynamice chemických reakcí a nelinearitě funkčních vztahů mezi vstupy a výstupy proměnných, vyžaduje řízení chemických procesů inteligentní kontrolu. „Chemický reaktor“ je jednou z hlavních procesních jednotek v chemickém, farmaceutickém a petrochemickém průmyslu, stejně jako v inženýrství řízení odpadu a životního prostředí. Navzdory pokračujícím pokrokům v rozvoji technik optimalizace a problémům řízení, stále existuje velká část příliš komplexních problémů, které se nedají řešit klasickými metodami.

Hlavním cílem této práce je demonstrovat fakt, že optimalizační nástroje, jakými jsou evoluční algoritmy (EA), mohou být použity pro prediktivní řízení a optimalizaci chemických procesů. V práci jsou použity čtyři algoritmy: Diferenciální evoluce (DE), Self organizing migrating algorithm (SOMA), Genetický algoritmus (GA) a Simulované žíhání (SA). V první části práce byly tyto evoluční algoritmy použity k optimalizaci parametrů dávkového reaktoru („batch reactor“). Následně jsou EA použity k modelování technických parametrů chemických reaktorů. Druhá část demonstruje optimalizaci chemických procesů, zvláště těch, ve kterých je použit evoluční algoritmus pro optimalizaci a řízení „Continuous stirred tank“ reaktorů.

Optimalizace a řízení chemických reaktorů byla provedena několika způsoby, každá pro jiný vektor parametrů reaktoru nebo s rozdílnou účelovou funkcí evolučního algoritmu. Veškeré optimalizované procesy jsou demonstrovány v grafech. Závěrem práce jsou prezentovány experimentální výsledky a jejich zhodnocení.

Klíčová slova: Optimalizace, Simulace, evoluční algoritmy, Batch, CSTR.

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LIST OF SYMBOLS AND ABBREVIATIONS

symbol	*unit*	*meaning*
EAs	-	evolutionary algorithms
EA	-	evolutionary algorithm
DE	-	differential evolution
SOMA	-	self-organizing migrating algorithm
GA	-	genetic algorithm
SA	-	simulated annealing
CSTRs	-	continuous stirred tank reactors
EP	-	evolutionary programming
ES	-	evolution Strategies
AGO	-	algorithms global optimization
$x_{i,G}$	-	individual in the current generation
$x'_{i,G}$	-	DE generates a new trial individual
$x_{r1,G}$, $x_{r2,G}$	-	randomly selected individuals
$u_{i,G+1}$	-	perturbation vector
G	-	current generation
δ	-	a random number
ΔE	-	the newly generated solution
$\dot{m}_{FK}$	[kg.s^{-1}]	mass flow rate of ”Input Chemical *FK*”
T_{FK}	[K]	temperature of ”Input Chemical *FK*”
c_{FK}	[J.kg. K^{-1}]	specific heat of ”Input Chemical *FK*”
$\dot{m}_V$	[kg.s^{-1}]	mass flow rate of “Input cooling medium”
T_{VP}	[K]	temperature of “Input cooling medium”
m_{VR}	[kg]	total weigh of jacketed through space of reaction
T_V	[K]	temperature of “output cooling medium”

c_V	[J.kg. K^{-1}]	specific heat of "output cooling medium"
m_P	[kg]	parameter mass initial batch inside the reactor
m	[kg]	total mass of reactionary mixture
T	[K]	temperature of reactionary mixture
c_R	[J.kg. K^{-1}]	specific heat of reactionary mixture
a_{FK}	[kmol m^{-3}]	concentration of chemical *FK*
A	[s^{-1}]	frequency factor
ρ_P	[kg.m^{-3}]	density of chemical *P*
K	[kg. s^{-3}. K^{-1}]	coefficient of heat transfer
ρ_{FK}	[kg.m^{-3}]	density of chemical *FK*
r	[m]	diameter of vessel
h	[m]	weight of vessel
ΔHr	[J. kg^{-1}]	heat of reaction
f_{cost}	-	cost function
PathLength	-	Control parameter of SOMA; it determines the stopping position of the movement of an individual
F	-	mutation constant
CR	-	constant of crossover
NP	-	number individuals of population in DE
Step	-	step size of migration
PRT	-	perturbation constant
PopSize	-	population size in SOMA
Migrations	-	number of rounds of migrations in SOMA
MinDiv	-	max. division values cost function of individuals sufficient for stopping algorithms
Individual Length	-	length of individuals
MutationCostant	-	mutation constant
Generations	-	number of generation cycles in DE
PocetCastic	-	number particle

DERan1Bin	-	strategy random version 1 Bin for DE
DERan2Bin	-	strategy random version 2 Bin for DE
SOMAATO	-	SOMA All to One
SOMAATR	-	SOMA All to One Random
SA_Elitism	-	strategy SA with Elitism
SA_NoElitism	-	strategy SA without Elitism
V_r	[m^3]	volume of the reactant mixture
V_c	[m^3]	volume of the coolant
Q_r	[$m^3 min^{-1}$]	volumetric flow rate of the reactant mixture
Q_c	[$m^3 min^{-1}$]	volumetric flow rate of the coolant
ρ_r	[kg m^{-3}]	density of the
ρ_c	[kg m^{-3}]	density of the the coolant
c_{pr}	[kJ $kg^{-1}K^{-1}$]	specific heat capacity of the reactant mixture
c_{pc}	[kJ $kg^{-1}K^{-1}$]	specific heat capacity of the coolant
A_r	[m^2]	heat exchange surface area
U	[kJ $m^{-2}min^{-1}K^{-1}$]	heat transfer coefficient
k_{10}, k_{20}	[m^{-1}]	pre-exponential factors
E_1, E_2	[K JKkmol^{-1}]	activation energies
R	[JKmol^{-1}]	gas constant
h_1, h_2	[kJ $kmol^{-1}$]	reaction enthalpies
c_{Ai}	[kmol m^{-3}]	concentration of chemical A for feed (inlet) value
c_{Bi}	[kmol m^{-3}]	concentration of chemical B for feed (inlet) value
T_{ri}	[K]	temperature of the reactant mixture (inlet)
T_{ci}	[K]	concentration of the coolant (inlet)
c_A^s	[kmol m^{-3}]	concentration of chemical A for steady-state value
c_B^s	[kmol m^{-3}]	concentration of chemical B for steady-state value

T_r^s	[K]	temperature of the reactant for steady-state value
T_c^s	[K]	temperature of the coolant for steady-state value

1 INTRODUCTION

The optimization of dynamic process has received growing attention in recent years because it is essential for the process industry to strive for more efficient and agile manufacturing in face of saturated market and global competition (T. Backx, O. Bosgra 2000).

Evolutionary algorithms such as evolution strategies and genetic algorithms have become the method of choice for optimization problems that are too complex to be solved using deterministic techniques such as linear programming or gradient (Jacobian) methods. The large number of applications (Beasley (1997)) and the continuously growing interest in this field are due to several advantages of EAs compared to gradient based methods for complex problems (Ivo F. Sbalzarini, Sibylle Muller and Petros Koumoutsakos 2000).

In chemical engineering, evolutionary optimization has been applied by the author and others to system identification (Pham and Coulter, 1995; Moros, 1996); a model of a process is built and its numerical parameters are found by error minimization against experimental data. Evolutionary optimization has been widely applied to the evolution of neural networks models for use in control applications (e.g. Li & Haubler, 1996).

The area of reactor network synthesis currently enjoys a proliferation of contributions in which researchers from various perspectives are making efforts to develop systematic optimization tools to improve the performance of chemical reactors. The contributions reflect on the increasing awareness that textbook knowledge and heuristics (Levenspiel, 1962), commonly employed in the development of chemical reactors, are now deemed responsible for the lack of innovation, quality, and efficiency that characterizes many industrial designs.

The main aim of this participation is to show that evolutionary algorithms (EAs) are capable of optimization on chemical engineering processes. The ability of EAs to successfully work with at investigation on optimization and predictive control of chemical reactors.

Firstly, a non-linear mathematical model is required to describe the dynamic behaviour of batch process; this justifies the use of evolutionary method of the EAs to deal with this process, for static optimization of a chemical batch reactor. Consequently, it is used to design geometry technique equipments for chemical reaction. The method was used to optimize the design of the growth chamber, and was found to be in good agreement with the observed growth rate results. The second one was chosen for optimization of a continuous stirred tank reactor (CSTR). On the next part, we have used EAs to predictive control of chemical process of rectors too.

The following and the biggest part describes the results of optimization of chemical process. The optimizations and control chemical reactors have been performed in several ways, each one for a different set of reactor parameters or different cost function. The optimized reactor and predictive control were used in a simulation with optimization by evolutionary algorithms and the results are presented in graphs.

This thesis is followed by a brief description of the chemical reactors and used EAs. Evolutionary algorithms are then studied, and finally experimental results are reported, followed by conclusion.

2 THE AIMS OF DISSERTATION

This dissertation aims to show how methods of artificial intelligence--mainly evolutionary computational techniques--can be used in dynamical systems of chemical reactors, particularly for the complex tasks of analyses and optimization of predictive control. The main focus here is on the examples of evolution algorithms (EAs) implementation in methods for achieving stable chemical reaction. The purpose is to obtain better results, meaning efficiency in reaching the desired stable state and superior stabilisation, through having robust and effective optimization of predictive control.

EAs is used to determine the optimal settings for the adjustable parameters, which are then used to achieve the desired state or behaviour of the chemical reactors' process. As noted in the results and conclusion of the presented project, EAs are able to find the optimal solution for the selected control technique. Thus avoiding complicated mathematical analysis of chemical process to find the settings for control method.

Research on this thesis is concerned with the field of optimization of chemical engineering through EAs. The main purposes and goals of the research can be summarised as thus:

1. Introduction of the chemical engineering process, formulation of the mathematical problems, and the description and analysis of the chosen dynamic systems--more concretely those in the processes of a Batch reactor and a Continuous stirred-tank reactor (CSTR);
2. Proposing a set of solving algorithms for the application of stochastic optimization, which enhances confidence in the optimization results, particularly in the chemical reaction;
3. Selecting and demonstrating EAs and practical method to optimize the chemical process, especially of Batch and CSTR reactors;

4. Demonstrating the use of designed algorithms for global optimization of the predictive control chemical processes and comparison between each selected algorithms; and
5. Presenting conclusions and suggesting further research perspective.

3 CHEMICAL ENGINEERING PROCESS

3.1 General introduction

The chemical industry produces many products by using chemical reaction and physical processes. To successfully realize these processes of chemical technology, it is necessary to make quantitative and qualitative analyses, especially in places where there is planned automated systems of technology processes control. To make the modernization of present and future processes purposeful, it is necessary to divide the modernization into periods.

The first and very important period is the analyzing of the industrial producing system. It usually includes simulations based on real model of chemical-physical processes for converting input sources into output products. These simulations will show the important key points of the technological process and where necessary changes to a new control system will be able to significantly improve the technological process's efficiency.

It is possible to say generally that the key technological points are the chemical reactors. To design the optimal parameters of reactor and its control system is one of the most difficult tasks of the process engineering. The situation is very often complicated by the imprecise kinetic principles of chemical reaction, which necessitates extensive measurements of dependencies of input and output elements on time, temperature, pressure, and etc. These quite complicated kinetic models (which are usually verified by experimental measurements) can be simplified using different methods into simpler models of which known methods of control already exist.

Notwithstanding the petrochemical industry, big attention must be paid to materials used in the production of macromolecular substances, i.e. plastic materials. Macromolecular substances are created from two kinds of reactions – polymerization and polycondensation. Algorithms must be designed to control these reactions, of which the majority comprises exothermic reactions (they produce heat). From an economic point of view, it is expected to have maximum efficiency of chemical reactor productivity with required quality. The reactor productivity depends on reacting speed, and reacting speed usually rises exponentially with temperature.

Although it may seem that the exothermal kind of reaction is a big advantage for us, it may not always be true due to security reasons and product quality (rising temperature may decrease the output product quality). The product quality may decrease especially in cases when the main reaction is followed by side reactions, their speed exponentially raised with temperature as well. As such, the most important parameter that has to be controlled during exothermic reactions is the reaction compound temperature. For this reason, the models presented in this work are based on enthalpy balances, with relevant simulations.

Nowadays, the application domain of chemical reactions and reactors constitutes one of the backbones for interdisciplinary collaboration. In fact, the optimization of industrial chemical processes has drawn attention in recent years. For experimental determination of the most important parameter - this thesis is described and analysed process of a Batch and Continuous stirred tank reactors. It is hoped that the examples presented here will provide some appreciation of the creative process.

3.2 Batch reactor

The Batch reactor is the generic term for a type of vessel widely used in the process industries. Its name is something of a misnomer since vessels of this type are used for a variety of process operations such as solids dissolution, product mixing, chemical reactions, batch distillation, crystallization, liquid/liquid extraction and polymerization. In some cases, they are not referred to as reactors but have a name which reflects the role they perform (such as crystallizer, or bio reactor).

The advantages of the batch reactor lie with its versatility. A single vessel can carry out a sequence of different operations without the need to break containment. This is particularly useful when processing, toxic or highly potent compounds.

3.2.1 Characteristics of batch processes

The optimization of batch processes has attracted attention in recent years (Aziz et al. 2000; Silva et al. 2003) because, in the face of growing competition, it is a natural choice for reducing production costs, improving product quality, meeting safety requirements and environmental regulations. Batch and semi-batch processes are of considerable importance in the fine chemicals industry. A wide variety of special chemicals, pharmaceutical products, and certain types of polymers are manufactured in batch operations. Batch processes are typically used when the production volumes are low, when isolation is required for reasons of sterility or safety, and when the materials involved are difficult to handle. In batch operations, all the reactants are charged in a tank initially and processed according to a pre-determined course of action during which no material is added or removed. In semi-batch operations, a reactant may be added with no product removal, or a product may be removed with no reactant addition, or a combination of both. From a process systems point of view, the key feature that differentiates continuous processes from batch and semi-batch processes is that continuous processes have a steady state, whereas batch and semi-batch processes do not (Srinisavan 2000 et al. 2002a and 2000b).

Reactor Configurations

In batch system all reactants are added to the tank at the given starting time. During the course of reaction, the reactant concentrations decrease continuously with time, and products are formed. On completion of the reaction, the rector is emptied, cleaned and is made ready for another batch.

This type of operation provides great flexibility with very simple equipment and allows differing reaction to be carried out in the same reactor. The disadvantages are the downtime needed for loading and cleaning and possibly the changing reaction conditions. Batch operation is often ideal for small scale flexible production and high value, low output product production, where the chemistry and reaction kinetics are not known exactly. In semi-batch operation, one reactant may be charged to the vessel at the start of the batch, and then the other fed to the reactor at perhaps varying rate and over

differing time periods. When the vessel is full, feeding is stopped and the contents allowed to discharge. Semi-batch operation allows one to vary the reactant concentration to a desired level in a very flexible way, and thus to control the reaction rates and the reactor temperature. It is, however, necessary to develop an appropriate feeding strategy. Modelling and simulation allows estimation of optimal feeding profiles. Sometimes it is necessary to adjust the feeding rates using feedback control. The flexibility of operation is generally similar to that of a batch reactor system. (J. Ingham, I.J.Dunn, E.Heinzle, J.E.P 2000).

Heat transfer to and from reactor

Heat transfer is usually affected by coils or jackets, but can also be achieved with the use of external loop heat exchanger and, in certain case; heat is transported out of the reactor. The treatment here mainly concerns jackets and coils.

Fig. 1. Batch reactor with single external cooling jacket

3.3 Continuous stirred tank reactors (CSTR)

The continuous stirred-tank reactor (CSTR), also known as vat- or back mix reactor is a common ideal reactor type in chemical engineering. A CSTR

often refers to a model used to estimate the key unit operation variables when using a continuous agitated-tank reactor to reach a specified output.

CSTR runs at steady state with continuous flow of reactants and products; the feed assumes a uniform composition throughout the reactor, exit stream has the same composition as in the tank.

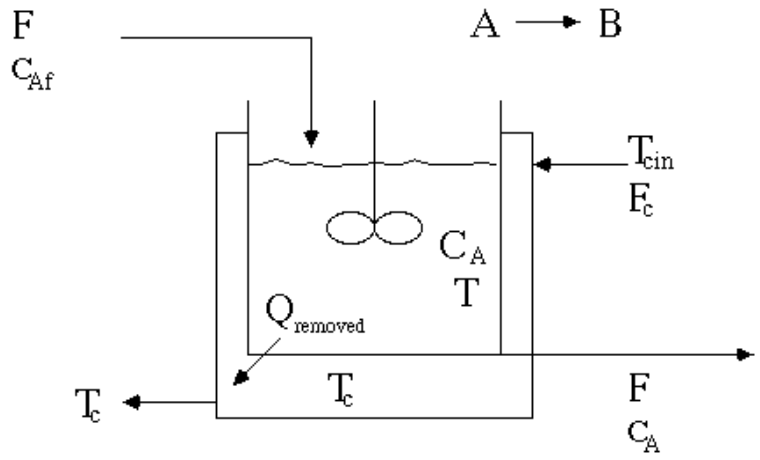


Fig. 2. Scheme of Continuous Stirred Tank Reactor with Cooling Jacket

where A is the raw material, B is the desired product, and C is an undesired by-product.

3.3.1 Characteristics of CSTR process

Continuous stirred tank reactors (CSTRs) belong to a class of nonlinear systems where both steady-state and dynamic behaviour are nonlinear. Their models are derived and described in e.g. (Ogunnaike and Ray, 1994), (Schmidt, 2005) and (Corriou, 2004). verification can be found in (Stericker and Sinha, 1993).

Chemical process control requires intelligent monitoring due to the dynamic nature of the chemical reactions and the non-linear functional relationship between he input and output variables involved. CSTR is one of

the major processing unit in many chemical, pharmaceutical and petroleum industries as well as in environmental and waste management engineering. In spite of continuing advances in optimal solution techniques for optimization and control problems, many of such problems remain too complex to be solved by the known techniques (Emuoyibofarhe O.Justice, Reju A Sunday, 2008).

4 METHODS AND EVOLUTIONARY ALGORITHMS

4.1 Introduction and a brief survey to Evolutionary Algorithms

As the history of the field suggests there are many different variants of Evolutionary Algorithms. The common underlying idea behind all these techniques is the same: given a population of individuals the environmental pressure causes natural selection (survival of the fittest) and this causes a rise in the fitness of the population. Given a quality function to be maximised we can randomly create a set of candidate solutions, i.e., elements of the function's domain, and apply the quality function as an abstract fitness measure – the higher the better. Based on this fitness, some of the better candidates are chosen to seed the next generation by applying recombination and/or mutation to them. Recombination is an operator applied to two or more selected candidates (the so-called parents) and results one or more new candidates (the children). Mutation is applied to one candidate and results in one new candidate. Executing recombination and mutation leads to a set of new candidates (the offspring) that compete – based on their fitness (and possibly age)– with the old ones for a place in the next generation. This process can be iterated until a candidate with sufficient quality (a solution) is found or a previously set computational limit is reached. In this process there are two fundamental forces that form the basis of evolutionary systems.

Variation operators (recombination and mutation) create the necessary diversity and thereby facilitate novelty, while Selection acts as a force pushing quality.

The combined application of variation and selection generally leads to improving fitness values in consecutive populations. It is easy (although somewhat misleading) to see such a process as if the evolution is optimising, or at least "approximising", by approaching optimal values closer and closer over its course. Alternatively, evolution it is often seen as a process of adaptation. From this perspective, the fitness is not seen as an objective function to be optimised, but as an expression of environmental requirements. Matching

these requirements more closely implies an increased viability, reflected in a higher number of offspring. The evolutionary process makes the population adapt to the environment better and better.

Let us note that many components of such an evolutionary process are stochastic. During selection fitter individuals have a higher chance to be selected than less fit ones, but typically even the weak individuals have a chance to become a parent or to survive. For recombination of individuals the choice of which pieces will be recombined is random. Similarly for mutation, the pieces that will be mutated within a candidate solution, and the new pieces replacing them, are chosen randomly. The general scheme of an Evolutionary Algorithm can is given in Fig. 3 in a pseudo-code fashion. (A.e. Eiben and j.e. Smith, 2003).

```
BEGIN
  INITIALISE population with random candidate
solutions;
  EVALUATE each candidate;
  REPEAT UNTIL ( TERMINATION CONDITION  is satisfied )
DO
     1 SELECT  parents;
     2 RECOMBINE  pairs of parents;
     3 MUTATE  the resulting offspring;
     4 EVALUATE  new candidates;
     5 SELECT  individuals for the next generation;
  OD
END
```

Fig. 3. The general scheme of an Evolutionary Algorithm in pseudo-code

Structure of a population evolutionary algorithm show in Fig. 4. & 5.

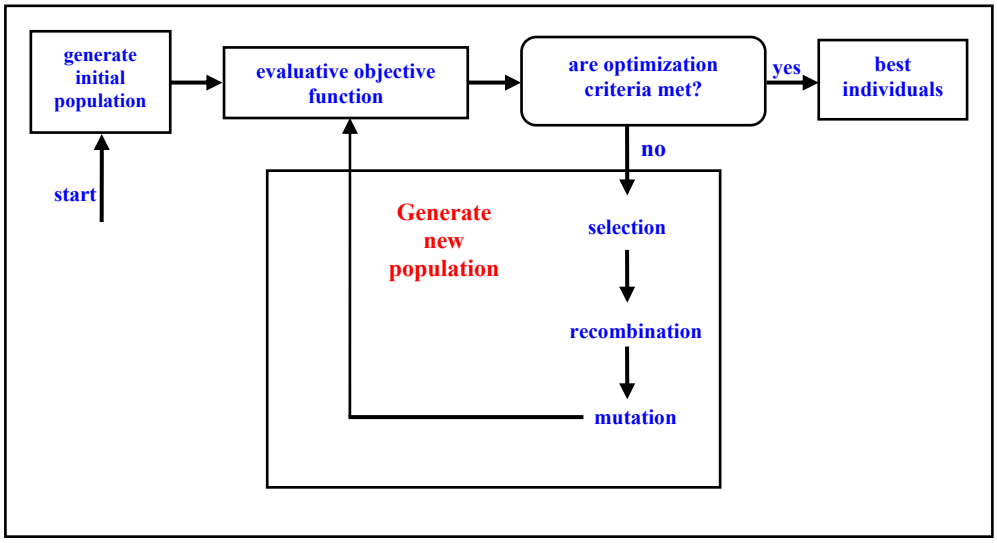


Fig. 4. Structure of a single population evolutionary algorithm

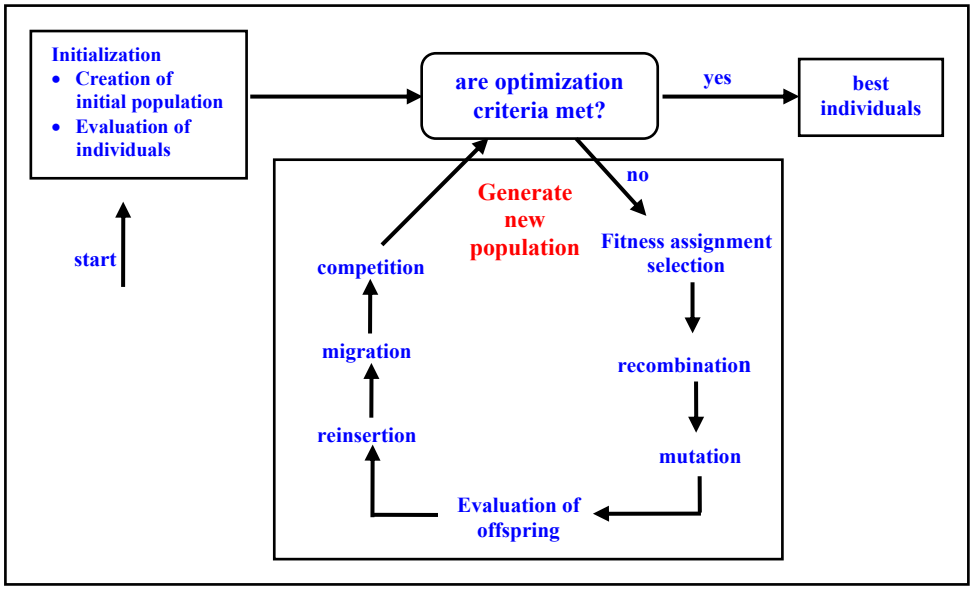


Fig. 5. Structure of an extended multipopulation evolutionary algorithm

Overview from source: http://www.geatbx.com/docu/algindex-01.html

According to (Zelinka, 2008) that extremely simply said, EA is a numerical process, during which N possible solutions of a given problem are processed together. These solutions are called "individuals" and are usually represented by a vector consisting of arguments of a defined cost function. A set of individuals (their number is called population size, which is the above-mentioned N) is called "population" and each individual is attached with a "fitness" , which can be in the simplest case the value of the cost function indicative of their suitability. For example, let us have a function Fcost (p1, p2, p3, p4, p5), then an individual is a set of parameters p, i.e. I={p1, p2, p3, p4, p5}, the population consists of N individuals with numerical values instead of x, like I1={2, 44, 51, −3.24, −22, 2}, I2, I3, …, IN={0.22, 3.4, 44, 1, 0.001, 0} (see Fig. 6). Parameter values in the individuals are assigned randomly at the beginning of the evolutionary process, i.e. the whole population is randomly generated. The population is then used to create the so-called offspring—new individuals, by means of selected individuals from a population (also called parents). This is done by operations like crossover, mutation, etc. A number of various variants of such operations are available because of the presence of a rich family of EAs. However, in principle, these operations are, in fact, arithmetical (or geometrical) operations, which combine selected individuals from a parental population.

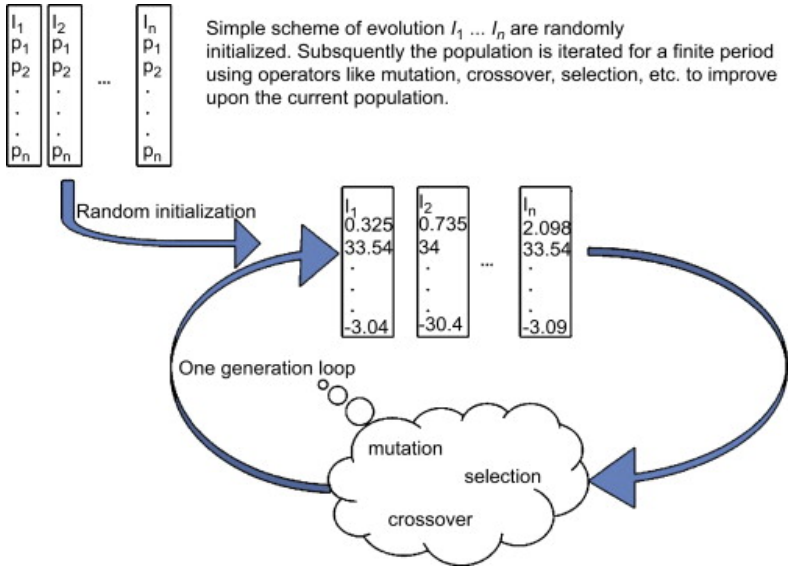


Fig. 6. Population in the evolutionary algorithm

Evolutionary process is thus an iterative process with the selection and survival of the temporarily best solutions, which are used in the next generation to create better solutions.

Finally, the best individual (i.e. problem solution) is selected from the last population and is regarded like the best solution from the actually ended evolution. The cost function used in the population should be defined so that its minimization or maximization should lead to the optimal solution. From this point of view, evolution can be also regarded like a mutually parallel search of an N-dimensional, nonlinear and complicated surface, where each point represent a possible solution. Example of the "cost function landscape" of the individual with two parameters, I={x, y} is depicted in Fig. 7 (see also Zelinka, 2004). Cost value is on the axis "z".

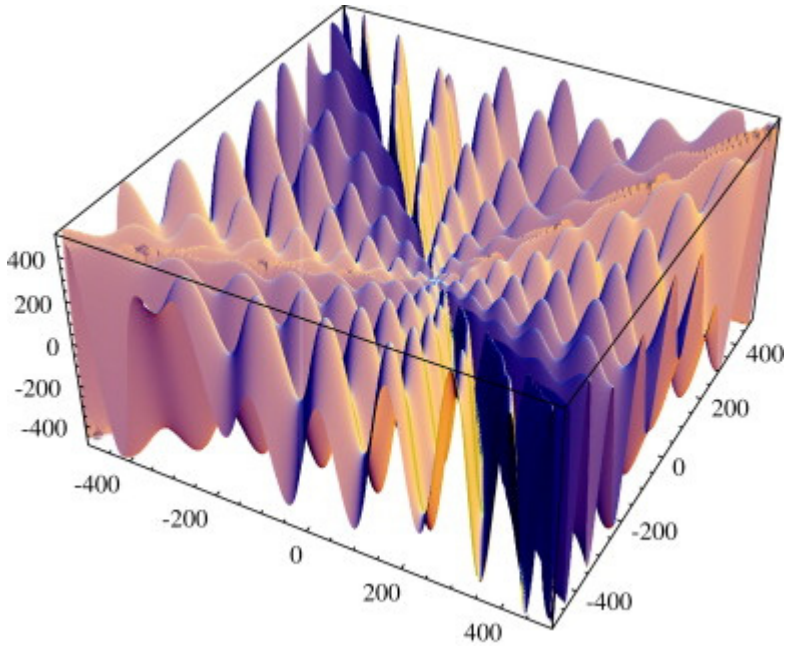


Fig. 7. Cost function surface representation, called Rana's function.

Today, a rich set of various versions of EAs exists. They differ by mathematical principles driving their evolutionary process as well as by the

fundamentally unique terminology and algorithm philosophy employed. Another difference is also that of individual representation, i.e. an individual can consist of integer or/and real numbers like I={2, 44, 51, −3.24, −22, 2} or can be based on binary string I={0010101101010101}, which is typical for genetic algorithm (GA) in its canonical version.

For a closer and more detailed study of EAs, which is time-consuming, it is recommended to use the literature like, for example, Holland (1975) and Davis (1996) (GAs), (Price, 1994), (Price, 1996) and (Price, 1999) (differential evolution (DE)), Kirkpatrick et al. (1983) and Cerny (1985) (simulated annealing (SA)), Eberhart and Kennedy (1995) and Clerc (2006) (particle swarm), Zelinka, (2004) (self-organizing migrating algorithm (SOMA)), Beyer (2001) (evolutionary strategies (ES)), Dorigo and Stützle (2004) (ant colony optimization), or in general Back et al. (1997).

4.2 A brief survey of Scoping and Screening chemical reaction networks using stochastic optimization

Many methods were adapted for the so-called optimal chemical reactors. The new methods focus on a systematic and thorough consideration of the available options and employ technology in the form of superstructures, optimization techniques, and a variety of graphical methods.

The importance of mathematical methods in optimizing reactors has been exemplified early enough with the application of dynamic programming for the estimation of optimal operating conditions in CSTR cascades (Aris, 1960) and the development of graphical techniques for single reversible reactions in PFRs (1961).

Around the same time, a set of brilliant contributions by Horn (1964) provided the basis of material that later emerged as attainable-region (AR) approaches. Dyson and Horn (1967) developed graphical tools for optimal temperature control schemes, feed distribution profiles along a PFR and catalyst minimization problems (Dyson and Horn, 1969). In these early days, separate groups made attempts to consolidate options and alternatives within comprehensive reactor structures (Ng and Rippin, 1965; Jackson, 1968;

Ravimohan, 1971). Optimization approaches initially addressed fixed reactor structures. Examples include the work of Paynter and Haskins (1970), and Chitra and Govind (1981, 1985a,b). The first studies of comprehensive structures should be attributed to Achenie and Biegler (1986, 1988, 1990), who employed existing representations (Jackson, 1968; Ng and Rippin, 1965) to launch optimization techniques in the form of NLP methods.

Kokossis and Floudas (1990, 1991, 1994) first introduced the idea of a reactor network superstructure modeled and optimized as an MINLP formulation. Though general and inclusive, their representation did not follow previous developments, but made an effort to facilitate the functionalities of the MINLP technology with the synthesis objectives. Mainly to scope, optimize and analyze the reaction process, Kokossis and Floudas replaced detailed models with simple though generic structures, enough to screen for design options and estimate the limiting performance of the reaction system. In the same vane, dynamic components have been replaced by CSTR cascades. A superstructure of generic elements (ideal CSTRs and PFRs) was postulated to account for all possible interconnections among the units. The representation was modeled and optimized as a MINLP model.

Though fundamental limitations appear evident, persistent efforts to extend the graphical methods have appeared in the literature (Hildebrandt et al., 1990; Hildebrandt and Glasser, 1990; Glasser et al., 1992, 1994; Feinberg and Hildebrandt, 1997; Price et al., 1997; Glasser and Hildebrandt, 1997; Hopley et al., 1996; Nisoli et al., 1997; McGregor et al., 1999; Godorr et al., 1999.)

A more promising direction has been pursued by Biegler and coworkers. The motivation has been to instill better guarantees in the optimization efforts by exploiting ideas and rules established in the construction of the AR. Applications presented in this area include the work by Balakrishna and Biegler (1992a,b) and Lakshmanan and Biegler (1994, 1996, 1997), and involved mathematical programming applications in the form of NLP and MINLP formulations. Optimal control formulation has been presented by Rojnuckarin et al. (1996) and Schweiger and Floudas (1999). Hildebrandt and Biegler (1994) presented a review of the attainable region approaches and suggested areas for future development of the concept. (Marcoulaki and Kokossis, 2004).

Especially in recent years, the methods of artificial intelligence, namely the evolutionary algorithms were used to optimise successfully chemical processes.

The optimization of non-linear constrained problems is relevant to chemical engineering practice [Wong, (1990); Salcedo, (1992); Floudas, (1995)]. Nonlinearities are introduced by process equipment design relations, by equilibrium relations and by combined heat and mass balances. The design variables may be floating points [non-linear programming (NLP) problems] or some of them may be integers [mixed integer non-linear programming (MINLP) problems].

In recent years, evolutionary algorithms (EAs) have been applied to the solution of NLP in many engineering applications. The best-known algorithms in this class include Genetic Algorithms (GA), Evolutionary Programming (EP), Evolution Strategies (ES) and Genetic Programming (GP). There are many hybrid systems, which incorporate various features of the above paradigms and consequently are hard to classify, which can be referred just as EC methods Dasgupta and Michalewicz, (1997). They differ from the conventional algorithms since, in general, only the information regarding the objective function is required. In recent years, EC methods have been applied to a broad range of activities in process system engineering including modeling, optimization and control. See for example real-time control of plasma reactor (Nolle et al., 2001 and (Nolle et al., 2005); Zelinka and Nolle, 2006), Optimization and control of batch reactor by evolutionary algorithms Senkerik, Zelinka, 2005], Optimization of reactive distillation processes using Self-organizing Migrating Algorithm and Differential Evolution Strategies (Tran, Zelinka, 2008), Using method of artificial intelligence to optimise and control chemical reactor (Tran, Zelinka, 2009), Investigation on optimization of Process Parameters and chemical reactor geometry by evolutionary algorithms (Tran, Zelinka, 2009) or An optimum solution for a process control problem (continuous stirred tank reactor) using a hybrid neural network (Emuoyibofarhe O.Justice, Reju A Sunday, 2008)…

4.3 Select Evolutionary Algorithms

For the experiments described here, stochastic optimisation algorithms, such as Differential Evolution (DE) (Price, 1999), Self-Organizing Migrating Algorithm (SOMA) (Zelinka, 2004), Genetic Algorithms (GA) (Holland, 1975) and Simulated Annealing (SA) (Kirkpatrick et al., 1983; Cerny, 1985) were selected. Main reason why DE, SOMA, GA and SA have been seed comes from contemporary state in chemical engineering and EAs use. Since now has been done some research with attention on use of EAs in chemical engineering optimization, including DE. This participation has to show that applicability of relatively new algorithms is also positive and can lead to applicable results, as was shown for example in Zelinka (2001), which has been done under 5th EU project RESTORM (acronym of Radically Environmentally Sustainable Tannery Operation by Resource Management) and main aim was to use EAs in chemical engineering processes. True is also that there is a plenty of other heuristic like particle swarm (Liu, Liu, Cartres, 2007), scatter search (Glover, Laguna, Martí, 2003), memetic algorithms, simulated annealing (Kirkpatrick, Gelatt, Vecchi, 1983), etc. and according to No Free Lunch teorem (Wolpert, Macready, 1997) is clear that each heuristic would be less or more applicable on example presented here. SOMA is a stochastic optimization algorithm that is modelled on the social behaviour of co-operating individuals (Zelinka, 2004). It was chosen because it has been proved that the algorithm has the ability to converge towards the global optimum (Zelinka, 2004). GA is one of the most modern paradigms for general problem solving. Genetic algorithms are more robust than existing directed search methods. Another important property of GA based search methods is that they maintain population of potential solutions – all other methods process a single point of the search space like hill climbing method. Hill climbing methods provide local optimum values and these values depend on the selection of starting point. Also there is no information available on the relative error with respect to global optimum. To increase the success rate in hill climbing method, it is executed for large number of randomly selected different starting points. On the other hand, GA is a multi-directional search maintaining a population of potential solutions and encourages information formation and exchange between these directions. Furthermore, SA is a generic probabilistic meta-algorithm for the global optimization problem,

namely locating a good approximation to the global optimum of a given function in a large search space. SA has been used in various combinatorial optimization problems and has been particularly successful in circuit design problems (see Kirkpatrick et al. 1983).

4.3.1 Differential Evolution (DE)

Differential Evolution (Price, 1999) (see Fig. 9) is a population-based optimization method that works on real-number coded individuals. For each individual $x_{i,G}$ in the current generation G, DE generates a new trial individual $x'_{i,G}$ by adding the weighted difference between two randomly selected individuals $x_{r1,G}$ and $x_{r2,G}$ to a third randomly selected individual $x_{r3,G}$. The resulting individual $x'_{i,G}$ is crossed-over with the original individual $x_{i,G}$. The fitness of the resulting individual, referred to as perturbated vector $u_{i,G+1}$, is then compared with the fitness of $x_{i,G}$. If the fitness of $u_{i,G+1}$ is greater than the fitness of $x_{i,G}$, $x_{i,G}$ is replaced with $u_{i,G+1}$, otherwise $x_{i,G}$ remains in the population as $x_{i,G+1}$. Deferential Evolution is robust, fast, and effective with global optimization ability. It does not require that the objective function is differentiable, and it works with noisy, epistatic and time-dependent objective functions. Pseudocode of DE shows:

$$
\begin{cases}
1.\ \text{Input} : D, G_{\max}, NP \geq 4, F \in (0,1+), CR \in [0,1], \text{and initial bounds} : \vec{x}^{(lo)}, \vec{x}^{(hi)}. \\
2.\ \text{Initialize} : \begin{cases} \forall i \leq NP \wedge \forall j \leq D : x_{i,j,G=0} = x_j^{(lo)} + rand_j[0,1] \bullet \left(x_j^{(hi)} - x_j^{(lo)}\right) \\ i = \{1,2,...,NP\},\ \ j = \{1,2,...,D\},\ G = 0,\ rand_j[0,1] \in [0,1] \end{cases} \\
\begin{cases}
3.\ \text{While} \quad G < G_{\max} \\
\begin{cases}
4.\ \text{Mutate and recombine} : \\
\qquad 4.1 \quad r_1, r_2, r_3 \in \{1,2,....,NP\}, \text{randomly selected, except} : r_1 \neq r_2 \neq r_3 \neq i \\
\qquad 4.2 \quad j_{rand} \in \{1,2,...,D\}, \text{randomly selected once each } i \\
4.3 \ \ \forall j \leq D, u_{j,i,G+1} = \begin{cases} x_{j,r_3,G} + F \cdot (x_{j,r_1,G} - x_{j,r_2,G}) \\ \qquad\qquad \text{if } (rand_j[0,1] < CR \vee j = j_{rand}) \\ x_{j,i,G} \quad \text{otherwise} \end{cases} \\
5.\ \text{Select} \\
\vec{x}_{i,G+1} = \begin{cases} \vec{u}_{i,G+1} & \text{if } f(\vec{u}_{i,G+1}) \leq f(\vec{x}_{i,G}) \\ \vec{x}_{i,G} & \text{otherwise} \end{cases}
\end{cases} \forall i \leq NP \\
G = G + 1
\end{cases}
\end{cases}
$$

Fig. 8. Pseudo code of DE

There are some version for optimization by mean differential evolution and two standard versions of DE, concretely DERand1Bin and DERand2Bin were chosen for optimization and predictive control of chemical reactors.

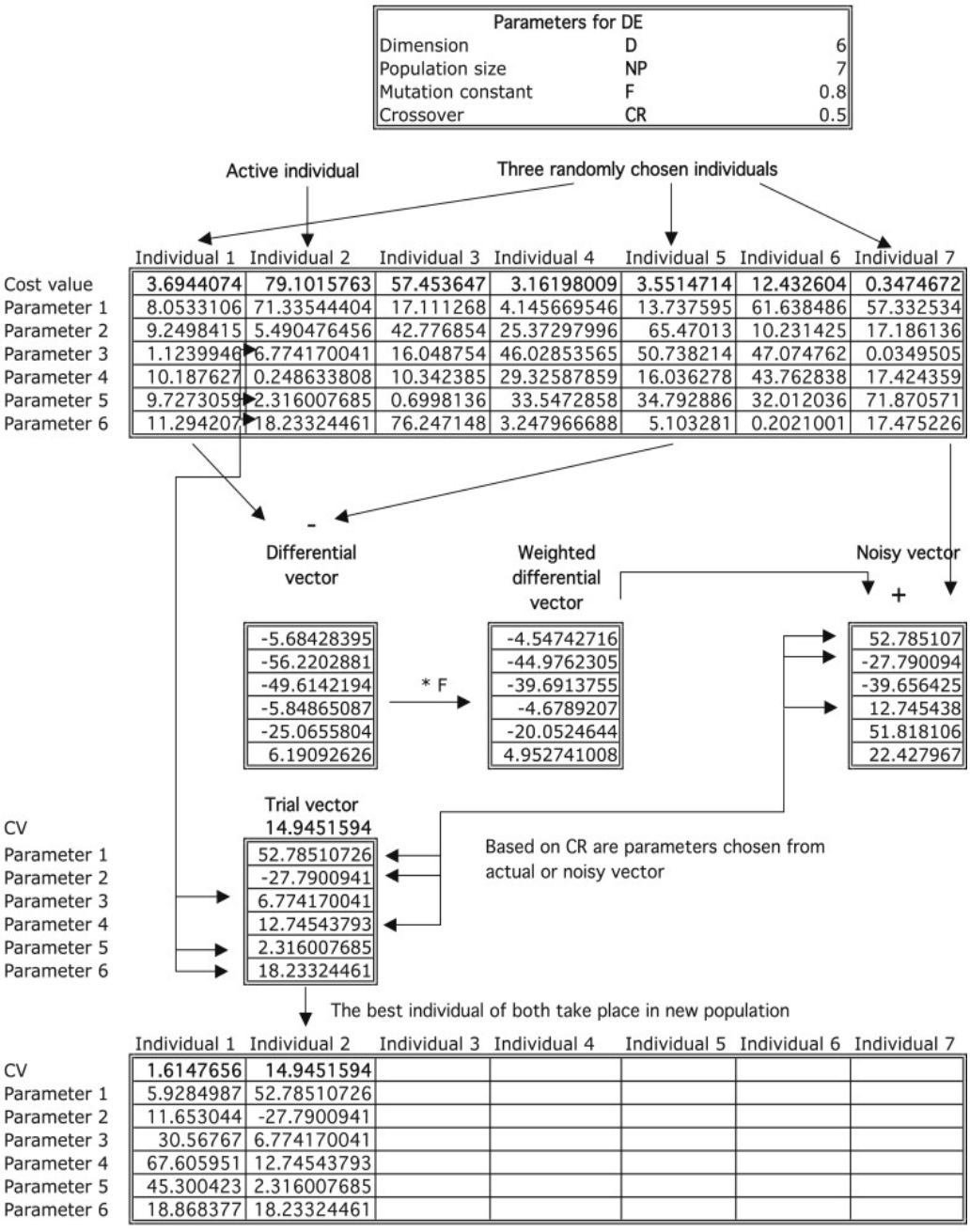


Fig. 9. Differential evolution, an artificial example (http://www.icsi.berkeley.edu/~storn/code.html).

4.3.2 Self Organizing Migrating Algorithm (SOMA)

SOMA is a stochastic optimization algorithm that is modelled on the social behaviour of co-operating individuals (Zelinka, 2004). It was chosen because it has been proved that the algorithm has the ability to converge towards the global optimum (Zelinka, 2004). SOMA works on a population of candidate solutions in loops called migration loops. The population is initialized randomly distributed over the search space at the beginning of the search. In each loop, the population is evaluated and the solution with the highest fitness becomes the leader L. Apart from the leader, in one migration loop, all individuals will traverse the input space in the direction of the leader. Mutation, the random perturbation of individuals, is an important operation for evolutionary strategies (ES). It ensures the diversity amongst the individuals and it also provides the means to restore lost information in a population. Mutation is different in SOMA compared with other ES strategies. SOMA uses a parameter called PRT to achieve perturbation. This parameter has the same effect for SOMA as mutation has for GA. The PRT Vector defines the final movement of an active individual in search space.

The randomly generated binary perturbation vector controls the allowed dimensions for an individual. If an element of the perturbation vector is set to zero, then the individual is not allowed to change its position in the corresponding dimension. An individual will travel a certain distance (called the path length) towards the leader in n steps of defined length. If the path length is chosen to be greater than one, then the individual will overshoot the leader. This path is perturbed randomly. For an exact description of use of the algorithms see (Price, 1999) for DE and (Zelinka, 2004) for SOMA. Pseudocode of SOMA shown in Fig. 10 and SOMA, an artificial example show in Fig. 11:

$$
\begin{aligned}
&\text{Input} : N, Migrations\ , PopSize \geq 2, PRT \in [0,1], Step \in (0,1], \text{MinDiv} \in (0,1], \\
&\qquad \text{PathLength} \in (0,5],\ Specimen \text{ with uper and lower bound } x_j^{(hi)}, x_j^{(lo)} \\
&\text{Inicialization} : \begin{cases} \forall i \leq PopSize \ \wedge \forall j \leq N : x_{i,j,Migrations\ =0} = x_j^{(lo)} + rand_j[0,1] \bullet \left(x_j^{(hi)} - x_j^{(lo)}\right) \\ i = \{1,2,...,Migrations\ \},\ j = \{1,2,...,N\},\ \text{Migrations} = 0,\ rand_j[0,1] \in [0,1] \end{cases}
\end{aligned}
$$

$$
\begin{cases}
\text{While}\ \ \text{Migrations} < Migrations_{\max} \\
\forall i \leq PopSize \begin{cases}
\text{While}\ \ t \leq PathLength \\
if\ rnd_j < PRT\ \ pak\ PRTVector_j = 1\ \ else\ 0, \quad j = 1,\ldots,N \\
x_{i,j}^{ML+1} = x_{i,j,start}^{ML} + (x_{L,j}^{ML} - x_{i,j,start}^{ML})\, t\, PRTVector_j \\
f\left(x_{i,j}^{ML+1}\right) = \text{ if } f\left(x_{i,j}^{ML}\right) \leq f\left(x_{i,j,start}^{ML}\right) \text{ else } f\left(x_{i,j,start}^{ML}\right) \\
t = t + Step
\end{cases} \\
\text{Migrations} = \text{Migrations} + 1
\end{cases}
$$

Fig. 10. Pseudocode of SOMA

Now a day, there are some versions of algorithms SOMA. In this work, I have used three strategies of SOMA for optimization and predictive control of chemical reactors. They are “All to One” (SOMAATO) and “All to One Random” (SOMAATR):

- **All to One** – this strategy was described in previous section. “All to one” means that all subjects in population migrate to the leader (except leader itself).
- **All to One Random** – is strategy, in which all individuals move back to one individual (Leader), which is not the deepest position on the hyperplane, but it is on the migration of individuals of each randomly selected from the population. Here emerged possible modification of this strategy, and such that the individuals don’t select randomly, but as appropriate, as is the case of genetic algorithms.

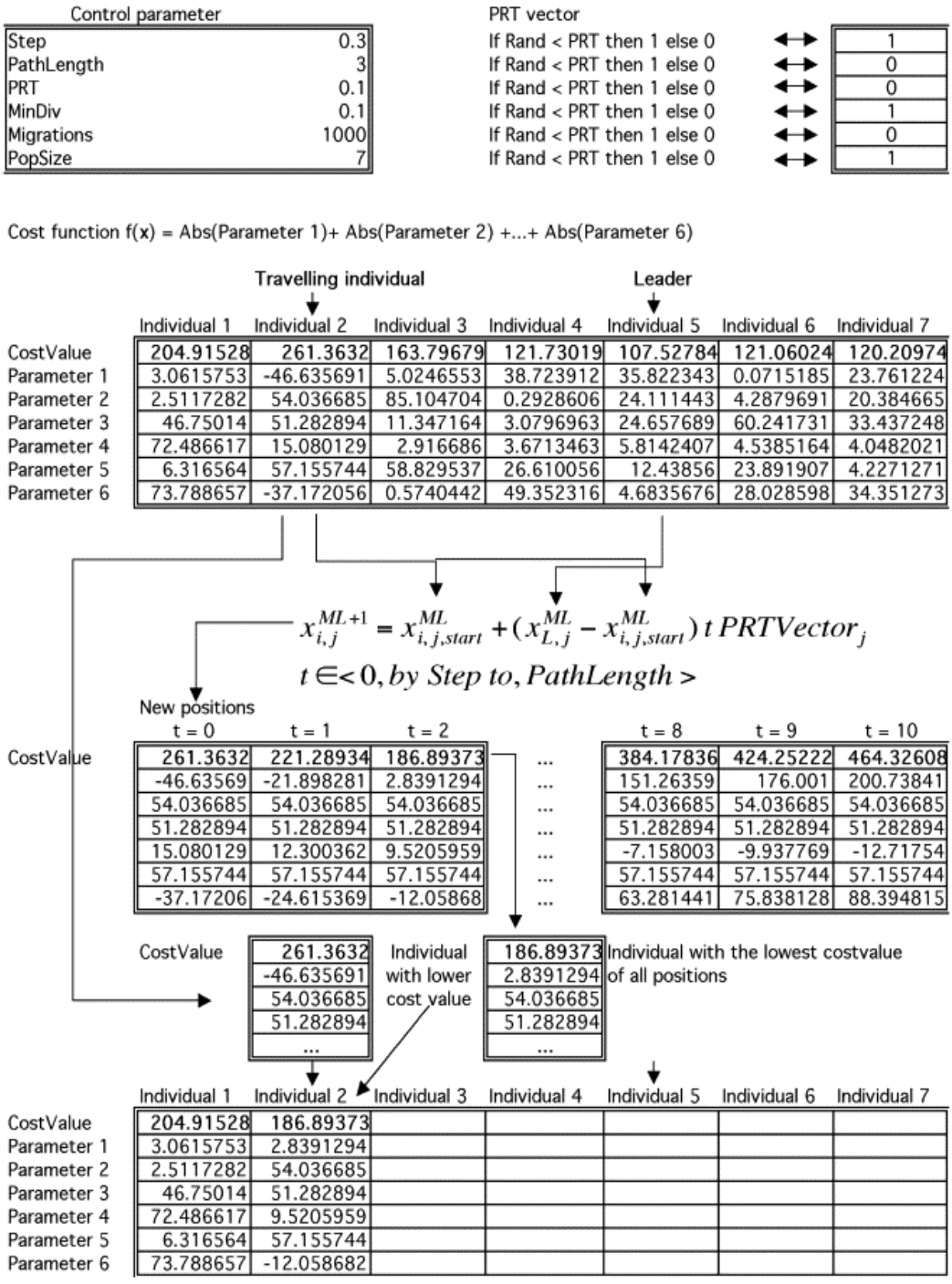


Fig. 11 . SOMA, an artificial example (http://www.fai.utb.cz/people/zelinka/soma).

4.3.3 Genetic Algorithm (GA)

Genetic Algorithms (GA) imitate the evolutionary processes with emphasis on genotype based operators (genotype/phenotype dualism). The GA works on a population of artificial chromosomes, referred to as individuals. Each individual is represented by a string of L bits. Each segment of this string corresponds to a variable of the optimizing problem in a binary encoded form.

The population is evolved in the optimization process mainly by crossover operations. This operation recombines the bit strings of individuals in the population with a certain probability Pc. Mutation is secondarily in most applications of a GA. It is responsible to ensure that some bits are changed, thus allowing the GA to explore the complete search space even if necessary alleles are temporarily lost due to convergence.

The following pseudocode describes the general principle of a Genetic Algorithm:

```
t = 0;
initialize(P(t=0));
evaluate(P(t=0));
while is NotTerminated() do
Pp (t) = P(t).selectParent();
Pc(t) = reproduction(Pp);
mutace(Pc(t));
evaluate(Pc(t));
P(t+1) = buildNextGenerationForm(Pc(t), P(t));
t=t+1;
end
```

Fig. 12. Pseudocode of GA (http://www.ra.cs.uni-tuebingen.de/software/EvA2/)

4.3.4 Simulated annealing (SA)

Simulated annealing (SA) is based on the similarity between the solid annealing process and solving combinatorial optimization problems (S. Kirkpatrick, C.D. Gelatt Jr and M.P. Vecchi,1983). SA consists of several decreasing temperatures. Each temperature has a few iterations. First, the beginning temperature is selected and an initial solution is randomly chosen.

The value of the cost function based on the current solution (i.e., the initial solution in this case) will then be calculated. The goal is to minimize the cost function. Afterwards, a new solution from the neighborhood of the current solution will be generated. The new value of the cost function based on the new solution will be calculated and compared to the current cost function value. If the new cost function value is less than the current value, it will be accepted. Otherwise, the new value would be accepted only when the Metropolis's criterion (N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller,1953), which is based on Boltzman's probability, is met. According to Metropolis's criterion, if the difference between the cost function values of the current and the newly generated solutions (ΔE) is equal to or larger than zero, a random number δ in [0,1] is generated from a uniform distribution. If Eq. (4.1) is met, the newly generated solution is accepted as the current solution.

$$\delta \leq e(-\Delta E/T) \tag{4.1}$$

The number of new solutions generated at each temperature is the same as the iteration number at the temperature which is constrained by the termination condition. The termination condition could be as simple as a certain number of iterations. After all the iterations at a temperature complete, the temperature would be lowered based on the temperature updating rule. At the updated (and lowered) temperature, all required iterations will have to be completed before moving to the next temperature. This process would repeat until the halting criterion is met. The halting criterion could be "reaching the pre-set minimum temperature." The result of simulated annealing (SA) is related to the number of iterations at each temperature and the speed of reducing temperature. The temperature updating rule proposed in this paper is shown in Eq. (4.2).

$$\text{Temperature} = Te^{(-rt)} \tag{4.2}$$

where T is the initial temperature, r the cooling ratio, and t the number of times the temperature has been lowered. The cooling ratio controls the speed of cooling. The higher the cooling ratio, the faster the temperature cools down.

Structure of simulated annealing algorithm show in Fig.13

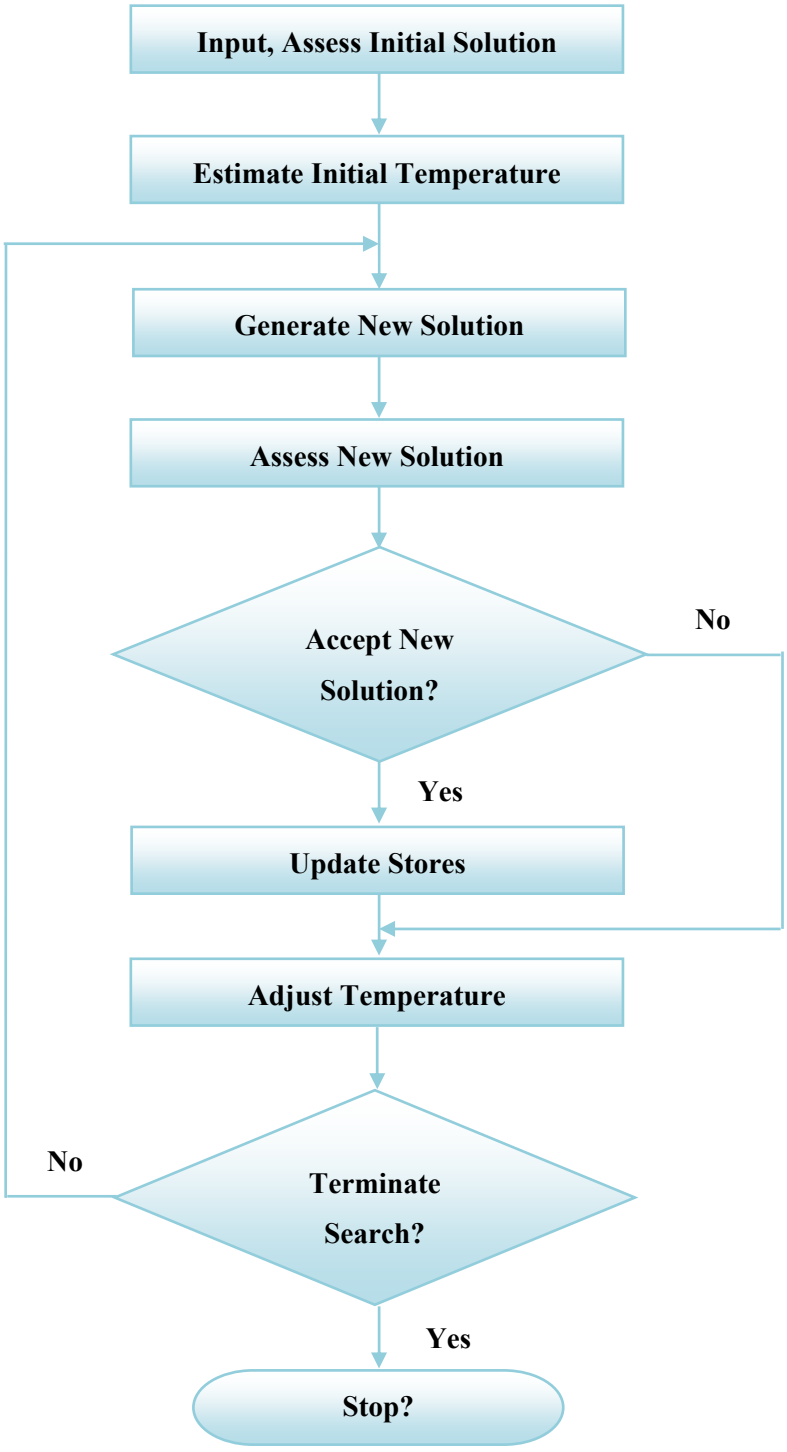


Fig. 13. Structure of simulated annealing algorithm

In this thesis I have chosen two versions of SA algorithms (SA elitism (SA_Elitism) and SA without elitism (SA_NoElitism)) for investigation on optimization and predictive control of a chemical reactor.

- **Usage of elitism**

It uses synchronization at the end of temperature phase, otherwise the communication proceeds asynchronous after each iteration.

- **Disadvantage** of this approach lies in excessive communication, which results in computation time increase.
- **Advantage** – elitism removes problem with the acceptance of worse solutions at low temperature phase

4.4 The cost function and principle simulation evolutionary algorithms in environment Mathematica

Evolutionary algorithms emerged as a mathematical analogy of the natural processes taking place in nature during evolution, which, if done completely at random, ensuring that they survive only individuals who are able to withstand the battle with the natural effect. This is the natural breeding population of individuals, when properties of the individual shall be amended so as to better accommodate natural conditions. This has become a fundamental principle of evolutionary algorithms to the initial randomly generated population of individuals forming a new generation of individuals with better characteristics, if appropriate, amending the parameters so that the values of cost function attained optimal values. Normally, therefore, looking for extreme function, usually a minimum, the *n*-dimensional hyperplane. Cost function of optimization problems can be specified as follows:

$$\min\left(f_{\cos t}\left(x\right)\right) \tag{4.3}$$

Using the optimal values of the arguments:

$$X = \left(x_1,...,x_D\right) \tag{4.4}$$

Where X is a vector composed of D parameters of cost function, they have limitations:

$$x_j^{(Lo)} \leq x_j \leq x_j^{(Hi)} \quad j = 1,\ldots,D \tag{4.4}$$

Where *Lo* is the lower limit, *Hi* is the higher limit.

Evolutionary algorithms (EAs) in environment mathematica perform according to a general cycle is illustrative in Fig. 14. Principle simulation evolutionary algorithms can be split into several steps: *Setting parameters and starting EAs, Generating population, Migration Process, Stop EAs and selecting the best individuals.*

Concretely, evolutionary algorithms SOMA will be governor through the following steps:

1. **Definition of parameters** - before running the algorithm it is necessary to select parameters such as: Step (step size of migration), *PathLength* (max distance migration), *MinDiv* (maximum division cost function values of individuals sufficient for stopping algorithms), *PopSize* (population size), *migration* (number of rounds of migration), *PRT* (constant perturbation), the *PRT* parameter is in some sense the equivalent of *CR* for parameter genetic algorithm and differential evolution. It has an impact on whether an individual will migrate directly to the leaders, or its trajectory will be diverted to the improved scanning n-dimensional space and thus to a higher robustness in finding global extreme. Without the use of *PRT* parameters SOMA often find only a local extreme .
2. **Generating population** - in this step is a randomly generated initial population in using the standard individual - *specimen*, which is precisely defined type and range of values <Lo, Hi> each of the individual parameters.
3. **Migration Process** - In this step, the actual migration of individual subjects after the n-dimensional hyperplane according to the rules of strategies SOMA algorithm.

4. **Evaluation** - At the end of the migration process is to evaluate the division cost function values of individual subjects. If this division is less than parameter *MinDiv*, the algorithm is ended - Step 5, otherwise the re-start the migration process - step 3.
5. **Stop algorithms SOMA and select the best individuals** of cost function values.

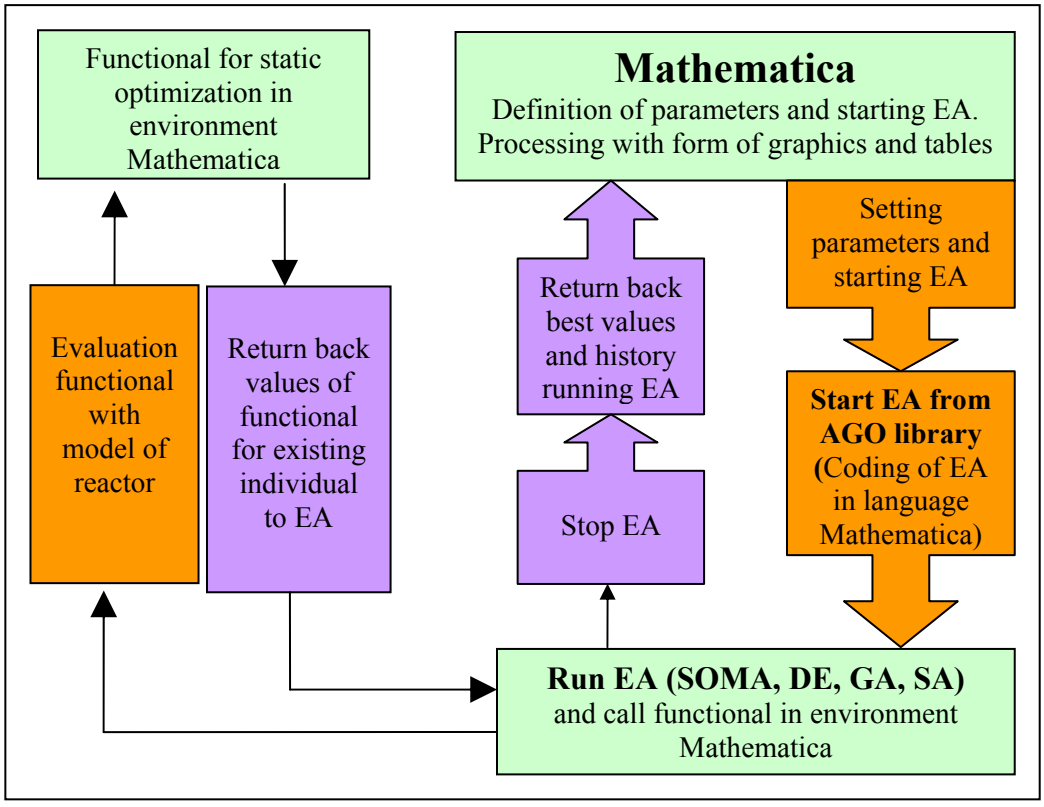


Fig. 14. Principle simulation evolutionary algorithms

From environment Mathemtica, I have created the "General subroutines call of SOMA, DE, GA, SA", which was shown in Fig. 15 and example for the overview process "Start EA" in environment Mathematica show in Fig. 16

```
StartEA[opt__] := Module[{pbest, pworst},
  ret = StringTake[ToString[opt], 2];
  FinalPopulation =Switch[ret,
  "SOMA",Population =
DoPopulation[PopSize,Specimen];Print["\nPopulation has
been initialized\n",Population // Transpose //
Tab.Form];CheckAbort[NestList[opt, Population,
Migrations], FinPop],
  "DE",Population =
DoPopulation[NP,Specimen];Print["\nPopulation has been
initialized\n",Population // Transpose //
Tab.Form];CheckAbort[NestList[opt, Population,
Generations], FinPop],
  "GA",Population =
DoGAPopulation[PopSize,Specimen];Print["\nPopulation has
been initialized\n",Population // Transpose //
Tab.Form];NestList[opt, Population, Generations],
  "SA",Population =
DoPopulation[PocetCastic,Specimen];Print["\nPopulation
has been initialized\n",Population // Transpose //
Tab.Form];StartSA[opt],
  _, Print["Unknown algorithm"]
];
    Print["\nFinal population is\n",
  Tab.Form[Transpose[Take[FinalPopulation, -1][[1]]]]];
      Print["\n"];
   BestInd[Take[FinalPopulation, -1][[1]]];
   Return[FinalPopulation]
]
```

Fig. 15. General subroutines call of SOMA, DE, GA, SA in environment Mathematica

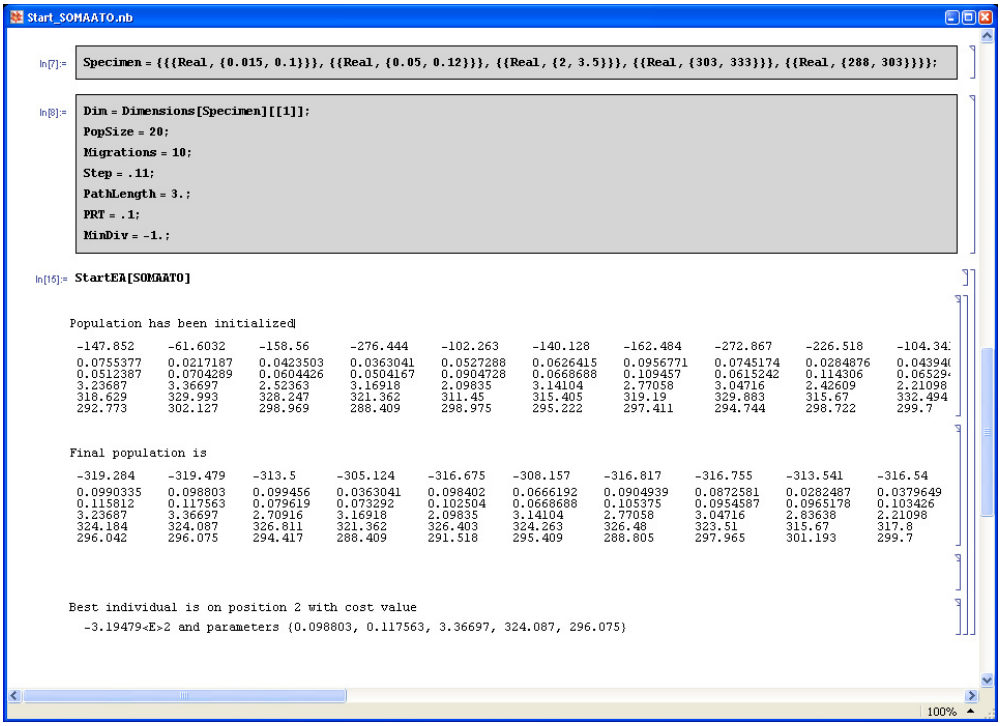


Fig. 16. Overview process "Start EA" in environment Mathematica (1x simulation of version SOMAATO)

4.4.1 Quality of the evolutionary processes

The quality and course of the evolutionary processes can be influenced by many factors, notably:

- **Setting parameters -** a combination of which may have a significant influence on the course and speed of evolution;
- **Population size -** a small population will limit choice while a major population will need more time to pass for the gradual creation of newer population;
- **Definition of cost function -** if badly or inappropriately defined, evolution may slow down to a stop;

- **Number of generations -** for a small number of generations, evolution may end before they find the extreme; and
- **Definition of the interval** - it is better to define the interval of evolution, and if there are uncertainties about, the evolutionary process can be maintained in the area of foreseeable solutions by looking at the extreme.

5 SIMULATION PART – PROBLEM DESIGN AND EXPERIMENTAL RESULTS

5.1 Introduction to simulation part

Presently, the chemical industry developes a wide range of products using a number of known physical and chemical laws in its chemical and technological processes. Quantitative and qualitative assessment should be done on these processes, particularly in the application of automated systems on the technological process, to ensure it is successfully managed.

Automated project management consist of several stages of which the most important step is the detailed analysis of the production systems. Evaluation on whether the system is in accordance with the description of its behaviour is done through simulation calculations performed on the computer. The calculations are based on the idea of the actual physical-chemical mechanisms, beginning with the original materials right through a defined sequence of events which eventually lead to the creation of the finished product with the desired characteristics and quality. The simulation calculations could help reveal key points of the technological process that needed modification through optimization techniques in order to meet the requirements of quality control with minimal production costs.

The application domain of the chemical reactions and reactors constitute one of the backbones for interdisciplinary collaboration. In fact, the optimization of industrial chemical processes has drawn attention in recent years, of which the optimal design and operation of chemical reactor is one of the most popular areas of study. The goal of this chapter is to show semirealistic design and optimization of chemical reactors processes, specifically of the Batch reactor and CSTR.

5.2 The main aim of chapter

This chapter's objective is to describe the implementation of optimization parameters of the Batch reactor and CSTR and the subsequent management of

the optimized reactors using the methods of artificial intelligence, namely EAs. Specifically, the algorithms are used to find the optimum parameters of the chemical reactor and model the technical requirements for chemical reaction. These tasks can be discussed within a few points:

- Development of a mathematical model of the process of chemical batch and CSTR reactor;
- Design optimization of the physical parameters of the reactor using EAs, i.e. finding appropriate cost functions, including the definition of its limitations and the implementation of the optimization using different versions of algorithms (SOMAATO, SOMAATR, DERan1Bin, DERan2Bin, GA, SA_Elitism, SA_NoElitism);
- The design of the reactor is based on standard chemical-technological methods and proposes a physical dimensions of the reactor and the parameters of the chemical substances. These values are known in this work as **expert parameters**. The objective of this part of the work is to perform a simulation and optimization of the given reactor.
- Evaluating and comparing the results obtained of each EA.

5.3 Optimization of batch reactor

5.3.1 Description of batch reactor

This work uses a mathematical model of a reactor shown in Fig. 17. From constructional standpoint, the acts about the vessel with double side for cooling medium and is further equipped with stirrer for mixing reactionary mixtures.

Reactor disposes by two physical inputs. First input denoted ”Input Chemical *FK*” is chemical dosing into reaction about mass flow rate $\dot{m}_{FK}$, temperature T_{FK} and specific heat c_{FK}. Second input denoted “Input cooling medium” is water drain into the reactor double side with mass flow rate $\dot{m}_V$, temperature T_{VP} and specific heat c_V. This coolant further traverses among -

jacketed through space of reaction and his total weight in this space is m_{VR}. Coolant after it gets off the exit reaction denoted "output cooling medium" about mass flow rate $\dot{m}_V$, temperature T_V and specific heat c_V. At the beginning of the process there is an initial batch inside the reactor with parameter mass m_P. Reactionary mixture then has total mass m, temperature T, specific heat c_R and stirs till the time chemicals *FK* described by parameter concentration a_{FK}.

This technique partially allows controlling the temperature of reaction mixture by the controlled feeding of the input chemical *FK*.

The main objective of optimization is to achieve the processing of large amount of chemical *FK* in a very short time. An exothermal reaction described by relationships (5.1) – (5.3) takes place in the reactor.

In general, this reaction is highly exothermal. Hence, the most important parameter is the temperature of the reaction mixture. **This temperature must not exceed 100°C** because of safety aspects and quality of the product.

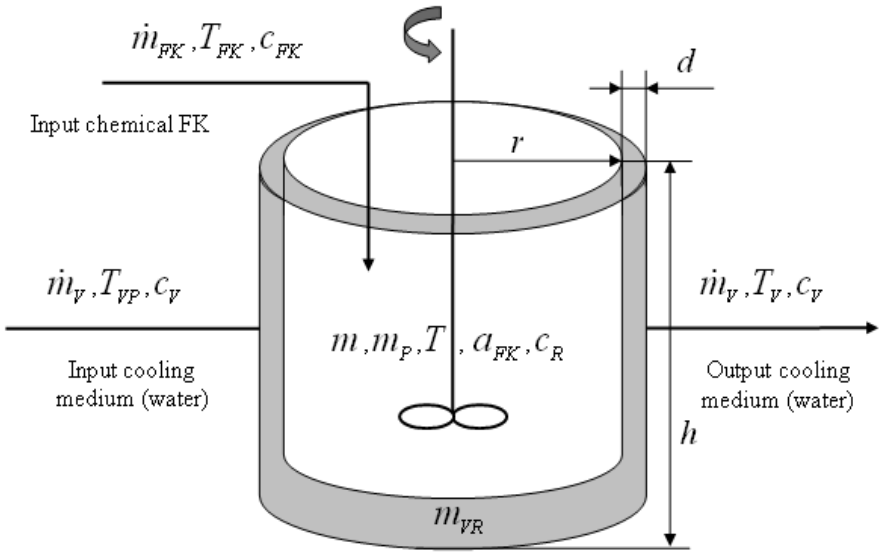


Fig. 17. Scheme Batch reactor

5.3.2 Problem design - Non-linear model of reactor

Description of the reactor applies a system of four balance equations (5.1). The first one expresses a mass balance of reaction mixture inside the reactor, the second a mass balance of the chemical *FK*, and the last two formulate entalpic balances, namely balances of reaction mixture and cooling medium.

Equation (5.1), in which (5.2) is represented by term "*k*", is written out here for simplified notation of basic equations.

$$\begin{aligned}
&\dot{m}_{FK} = m'[t] \\
&\dot{m}_{FK} = m[t]\, a'_{FK}[t] + k\, m[t]\, a_{FK}[t] \\
&\dot{m}_{FK} c_{FK} T_{FK} + \Delta H_r k\, m[t] a_{FK}[t] = K\, S\,(T[t] - T_V[t]) + m[t] c_R T'[t] \\
&\dot{m}_V c_V T_{VP} + K\, S\,(T[t] - T_V[t]) = \dot{m}_V c_V T_V[t] + m_{VR} c_V T'_V[t]
\end{aligned} \tag{5.1}$$

$$k = A e^{-\frac{E}{RT[t]}} \tag{5.2}$$

After modification into the standard form, the balance equations are obtained in form (5.3)

$$\begin{aligned}
&m'[t] = \dot{m}_{FK} \\
&a'_{FK}[t] = \frac{\dot{m}_{FK}}{m[t]} - A e^{-\frac{E}{RT[t]}} a_{FK}[t] \\
&T'[t] = \frac{\dot{m}_{FK} c_{FK} T_{FK}}{m[t] c_R} + \frac{A e^{-\frac{E}{RT[t]}} \Delta H_r a_A[t]}{c_R} - \frac{K S T[t]}{m[t] c_R} + \frac{K S T_V[t]}{m[t] c_R} \\
&T'_V[t] = \frac{\dot{m}_V T_{VP}}{m_{VR}} + \frac{K S T[t]}{m_{VR} c_V} - \frac{K S T_V[t]}{m_{VR} c_V} - \frac{\dot{m}_V T_V[t]}{m_{VR}}
\end{aligned} \tag{5.3}$$

The parameters for this reactor and initial conditions (a_{FK0}, T_{V0}, T_0, m_0, ...) were specified by expert, giving physical dimensions as well as parameters of individual chemical substances. These were used to simulate the behaviour of this reactor. The design of the reactor was based on standard chemical-technological methods and gives a proposal of reactor physical dimensions

and parameters of chemical substances. These values are called in this participation expert parameters. The objective of the work is to perform a simulation and optimization of the given reactor.

Therefore into system equations (5.3) were instated constants:

A = 219,588 s-1, E = 29967,5087 J.mol-1, R = 8,314 J. mol-1.K-1, cFK = 4400 J.kg. K-1, cV = 4118 J.kg. K-1, cR = 4500 J.kg. K-1, ΔHr = 1392350 J. kg-1, K = 200 kg. s-3. K-1.

Next parameters, that are important for calculations are:

- Geometric dimension of the reaction: r[m] , h[m]
- Density of chemicals: ρ_P = 1203 kg.m^{-3} , ρ_{FK} = 1050 kg.m^{-3}
- Stoicheiometric rate chemical: $m_P = 2{,}82236.m_{FK}$

5.3.3 *Optimization of process parameters and the reactor geometry*

The design approach using the batch reaction system show in Fig.18. The main aim in this example is finding the optimization of process parameters and the reactor geometry. Here, it is a optimization of batching value $\dot{m}_{FK}$ together with process parameters of the cooling medium and including also reactor geometry and cooling area.

Tab.1 Parameters of reactor, "yellow" was optimized

$\dot{m}_{FK} \rightarrow \frac{\text{Kilogram}}{\text{Second}}$	$\dot{m}_V \rightarrow \frac{\text{Kilogram}}{\text{Second}}$	$m_V \rightarrow$ Kilogram	$m_P \rightarrow$ Kilogram
$E \rightarrow \frac{\text{Joule}}{\text{Mole}}$	$R \rightarrow \frac{\text{Joule}}{\text{Mole Kelvin}}$	$A \rightarrow \frac{1}{\text{Second}}$	$\Delta H_r \rightarrow \frac{\text{Joule}}{\text{Kilogram}}$
$T_{FK} \rightarrow$ Kelvin	$T_{VP} \rightarrow$ Kelvin	$K \rightarrow \frac{\text{Kilogram}}{\text{Kelvin Second}^3}$	$T \rightarrow$ Kelvin
$c_{FK} \rightarrow \frac{\text{Joule}}{\text{KilogramKelvin}}$	$c_V \rightarrow \frac{\text{Joule}}{\text{Kilogram Kelvin}}$	$c_R \rightarrow \frac{\text{Joule}}{\text{Kilogram Kelvin}}$	$m \rightarrow$ Kilogram
$d \rightarrow$ Meter	$h \rightarrow$ Meter	$r \rightarrow$ Meter	$m_{VR} \rightarrow$ Kilogram

5.3.3.1 Mathematical problems

In this optimization was founded optimized parameters with one another linked ,so that heat transfer surface, volume, and hence also mass mixtures of reaction was mutually in relation. Heat transfer surface *S* has relation:

$$S = 2\pi rh + \pi r^2 \tag{5.4}$$

Where *r* is radius and *h* is high of the space reactor (see Fig.15)

Volume of vessel of rector applies to relation:

$$V = \pi r^2 h \tag{5.5}$$

Total mass of mixtures in the reaction is initial batch inside the reactor with parameter mass m_P a mass "input chemical *FK*" m_{FK} , that:

$$m = m_p + m_{FK} \tag{5.6}$$

The stechiometric ratio is given by (5.7).

$$m_P = 2{,}82236 m_{FK} \tag{5.7}$$

Total volume of mixtures in the reaction equal sum of volume initial mixtures in the reaction and volume of *FK*:

$$V = V_p + V_{FK} = \frac{m_p}{\rho_p} + \frac{m_{FK}}{\rho_{FK}} \tag{5.8}$$

The relationship between the optimized volume of reactor and the mass of added chemical *FK* is given by (5.8). Then substituting to (5.7) gives the mass of the initial batch in the reactor.

$$m_{FK} = \frac{\rho_p \rho_{FK} V}{2{,}82236\ \rho_{FK} + \rho_p} \tag{5.9}$$

In this example, the optimization was then added parameter thickness d of vessel, which have relation that:

$$m_{VR} = \rho_V Sd \tag{5.10}$$

5.3.3.2 The Cost Function (CF)

In this optimization the point was to minimize the area arising as a difference between the required and real temperature profile of the reaction mixture in a selected time interval, which was the duration of a batch cycle. The required temperature was 97°C (370.15 K). The cost function that was minimized is given in (5.11):

$$f_{\cos t} = \sum_{t=0}^{t} |w - T[t]| \tag{5.11}$$

Where: w - control point, T – temperature

The CF has been calculated in general from the distance between desired state and actual system output.

5.3.3.3 Parameter settings

The control parameter settings have been found empirically and are given in Tab. 2 (SOMA) and Tab. 3 (DE). In Tab. 4 and Tab. 5 are parameters setting for GA and SA. The main criterion for this setting was to keep the same setting of parameters as much as possible and of course the same number of cost function evaluations as well as population size (parameter PopSize for SOMA, GA and NP for DE). Number of optimized reactor parameters and their range inside represents in Tab. 6.

Tab.2 SOMA parameter setting

	A
PathLength	3
Step	0.41
PRT	0.1
PopSize	20
Migrations	50
MinDiv	-1
Individual Length	6
CF Evaluations	6951

Tab.3 DE parameter setting

	A
NP	20
F	0.9
CR	0.2
Generations	200
Individual Length	6
CF Evaluations	4000

Tab.4 GA parameter setting

	A
PopSize	20
MutationCostant	0.2
Generations	200
Individual Length	6
CF Evaluations	4000

Tab.5 SA parameter setting

	A
PocetCastic	2
diameter	0.5
kmax	66
Tmin	0.0001
Tmax	1000
alfa(cooling factor)	0.8

Tab.6 Optimized reactor parameters and their range inside which has been optimization done

Parameter	Range
$\dot{m}_{FK}$ [kg.s^{-1}]	0 – 500
r [m]	0.3 – 3.0
h [m]	0.5 – 3.5
T_{VP} [K]	273.15 – 323.15
$\dot{m}_{V}$ [kg.s^{-1}]	0-10
d [m]	0.03 – 0.1

5.3.3.4 Experimental Results

Due to the fact that EAs are partly of stochastic nature, a large set of simulations has to be done in order to get data for statistical data processing. Four algorithms (SOMA, DE, GA and SA) have been applied 100 times in order to find the optimum of process parameters and the reactor geometry. All important data has been visualized directly or/and processed for graphs demonstrating performance of four algorithms. Estimated parameters and their diversity (minimum, maximum and average) are depicted in Fig. 18 - Fig. 19. From those pictures it is visible that results from four algorithms are comparable. For the demonstration are graphically the best solutions show in Fig. 20 – Fig. 26 of items (*b), (d), (f), (h)*. There is shown time dependence of processes parameters from four algorithms. The best values of parameters setting are recorded in Tab.7 & Tab. 8. All one hundred simulations diversity (minimum, maximum and average) were described from Tab. 9 to Tab. 15 for each versions of four algorithms. On Fig. 20 – Fig. 26 are for example shown records of all 100 simulations and the best solutions of all 100 simulations (Fig. 20-21 for SOMA, Fig. 22 – 23 for DE, Fig. 24 for GA and Fig. 25-26 for SA).

Tab.7 The best values of optimized parameters by SOMA, DE

Parameter	SOMAATO	SOMAATR	DERan1Bin	DERan2Bin
$\dot{m}_{FK}$ [kg.s^{-1}]	0.0226579	0.0370397	0.225063	0.135087
r [m]	0.302427	0.496691	0.195776	2.50725
h [m]	3.12646	2.46924	0.83969	0.715263
T_{VP} [K]	319.286	311.758	296.179	318.115
$\dot{m}_{V}$ [kg.s^{-1}]	5.58697	9.57913	9.35465	9.431
d [m]	0.0474563	0.0379435	0.030377	0.0583956

Tab.8 The best values of optimized parameters by GA, SA

Parameter	GA	SA_Elitism	SA_NoElitism
$\dot{m}_{FK}$ [kg.s^{-1}]	0.00417218	0.187008	0.519387
r [m]	2.58293	2.51294	2.84268
h [m]	3.40438	0.858557	2.76458
T_{VP} [K]	310.944	314.657	319.494
$\dot{m}_{V}$ [kg.s^{-1}]	5.09912	9.02945	6.56782
d [m]	0.0315134	0.0597223	0.0918064

Parameter diversity for repeated 100 times simulations

Tab.9 Estimated parameters for DERand1Bin

Parameter	Min	Avg	Max
$\dot{m}_{FK}$ [kg.s^{-1}]	0.00732026	0.157858	0.467508
r [m]	0.360715	1.80667	2.97025
h [m]	0.506418	1.79237	3.47477
T_{VP} [K]	293.29	306.98	322.669
$\dot{m}_{V}$ [kg.s^{-1}]	5.32214	9.31932	9.99522
d [m]	0.0300719	0.0391487	0.078392

Tab.10 Estimated parameters for DERand2Bin

Parameter	Min	Avg	Max
$\dot{m}_{FK}$ [kg.s^{-1}]	0.0098592 4	0.133546	0.551649
r [m]	0.328569	1.48296	2.99652
h [m]	0.527274	1.96553	3.48392
T_{VP} [K]	293.185	306.886	323.001
$\dot{m}_{V}$ [kg.s^{-1}]	0.382172	8.31582	9.99879
d [m]	0.0300549	0.0440286	0.0941844

Tab.11 Estimated parameters for SOMAATO

Parameter	Min	Avg	Max
$\dot{m}_{FK}$ [kg.s^{-1}]	0.006463 0	0.029002 8	0.126721
r [m]	0.3	0.719769	2.38758
h [m]	0.500022	1.22914	3.29516
T_{VP} [K]	293.52	308.434	322.923
$\dot{m}_{V}$ [kg.s^{-1}]	2.91889	8.84481	9.99993
d [m]	0.030451 9	0.055827 9	0.0987916

Tab.12 Estimated parameters for SOMAATR

Parameter	Min	Avg	Max
$\dot{m}_{FK}$ [kg.s^{-1}]	0.015992 2	0.092730 6	0.378352
r [m]	0.321836	1.28136	2.88948
h [m]	0.501199	1.76971	3.47737
T_{VP} [K]	293.444	303.046	322.487
$\dot{m}_{V}$ [kg.s^{-1}]	1.66669	9.53494	9.99987
d [m]	0.030146 6	0.038627 4	0.093981

Tab.13 Estimated parameters for GA

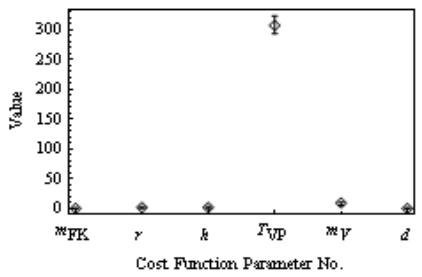
Parameter	Min	Avg	Max
$\dot{m}_{FK}$ [kg.s^{-1}]	0.0041721	0.362735	1.4908
r [m]	0.308429	2.20758	2.98134
h [m]	0.673105	2.2323	3.48275
T_{VP} [K]	293.253	308.797	323.114
$\dot{m}_{V}$ [kg.s^{-1}]	0.234471	5.14055	9.96397
d [m]	0.0303933	0.0652728	0.0995752

Tab.14 Estimated parameters for SA_Elitism

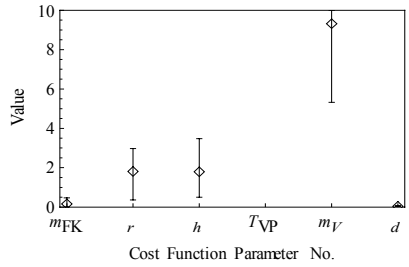
Parameter	Min	Avg	Max
$\dot{m}_{FK}$ [kg.s^{-1}]	0.0234063	0.25735	0.978476
r [m]	0.382136	2.12841	2.9857
h [m]	0.570715	2.25282	3.47805
T_{VP} [K]	293.557	309.318	322.894
$\dot{m}_{V}$ [kg.s^{-1}]	0.0981996	5.77572	9.99886
d [m]	0.0303382	0.0661099	0.0994636

Tab.15 Estimated parameters for SA_NoElitism

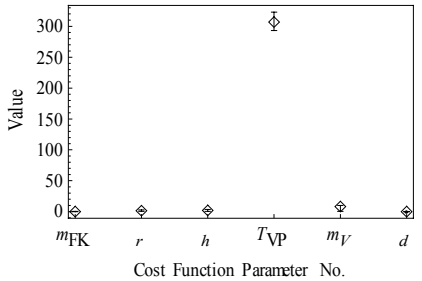
Parameter	Min	Avg	Max
$\dot{m}_{FK}$ [kg.s^{-1}]	0.0176978	0.315186	1.19071
r [m]	0.506012	2.1492	2.99712
h [m]	0.513602	2.30953	3.49055
T_{VP} [K]	293.282	306.615	322.332
$\dot{m}_{V}$ [kg.s^{-1}]	0.0015723	5.27791	9.90747
d [m]	0.0300534	0.0630213	0.0994389



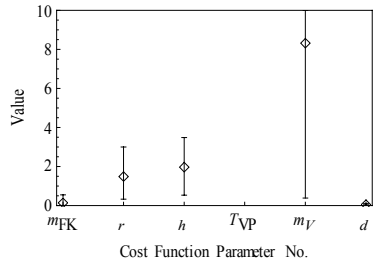
a) Parameter variation (DERan1Bin)



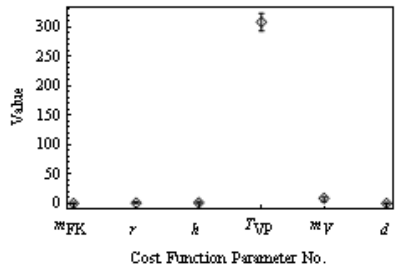
b)Parameter variation (DERan1Bin) – detail



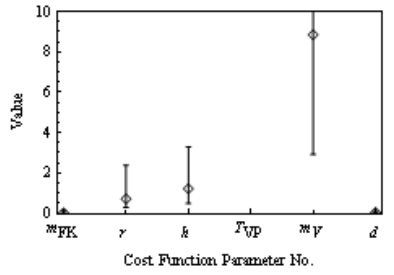
c) Parameter variation (DERan2Bin)



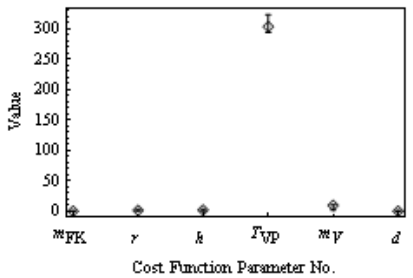
d).Parameter variation (DERan2Bin) – detail



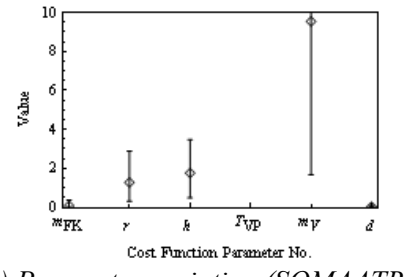
e) Parameter variation (SOMAATO)



f) Parameter variation (SOMAATO) – detail

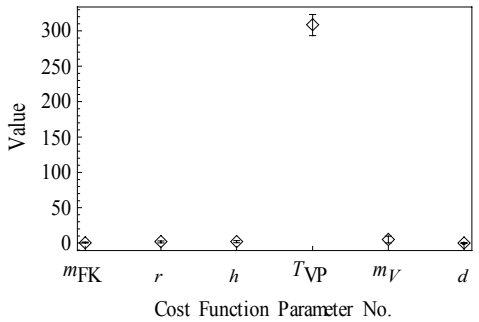


g) Parameter variation (SOMAATR)

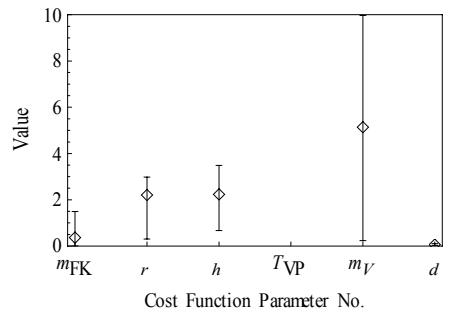


h) Parameter variation (SOMAATR) – detail

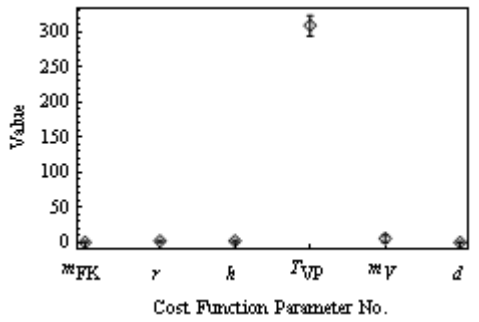
Fig. 18. Parameter variation of SOMA and DE



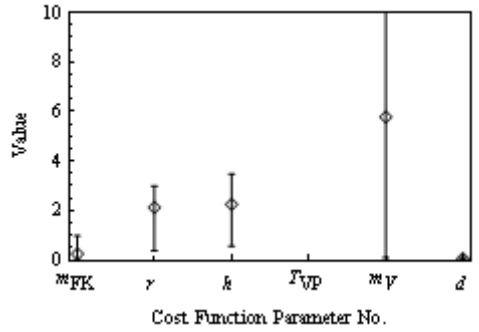
a) Parameter variation (GA)



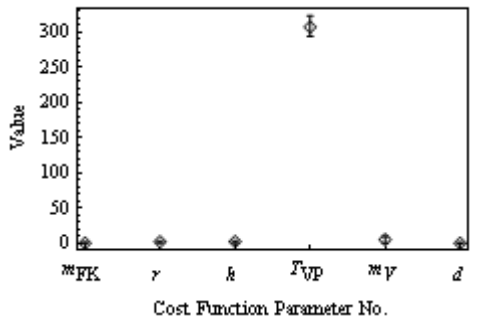
b) Parameter variation (GA) – detail



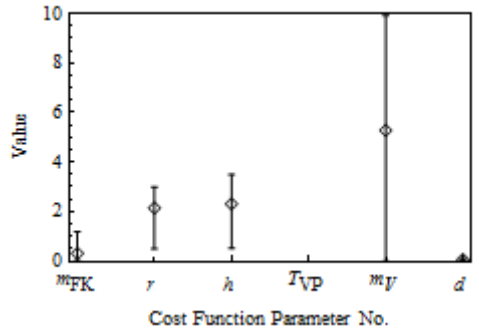
c) Parameter variation (SA_Elitism)



d) Parameter variation (SA_Elitism) – detail



e) Parameter variation (SA_NoElitism)



f)Parameter variation (SA_NoElitism) – detail

Fig. 19. Parameter variation of GA and SA

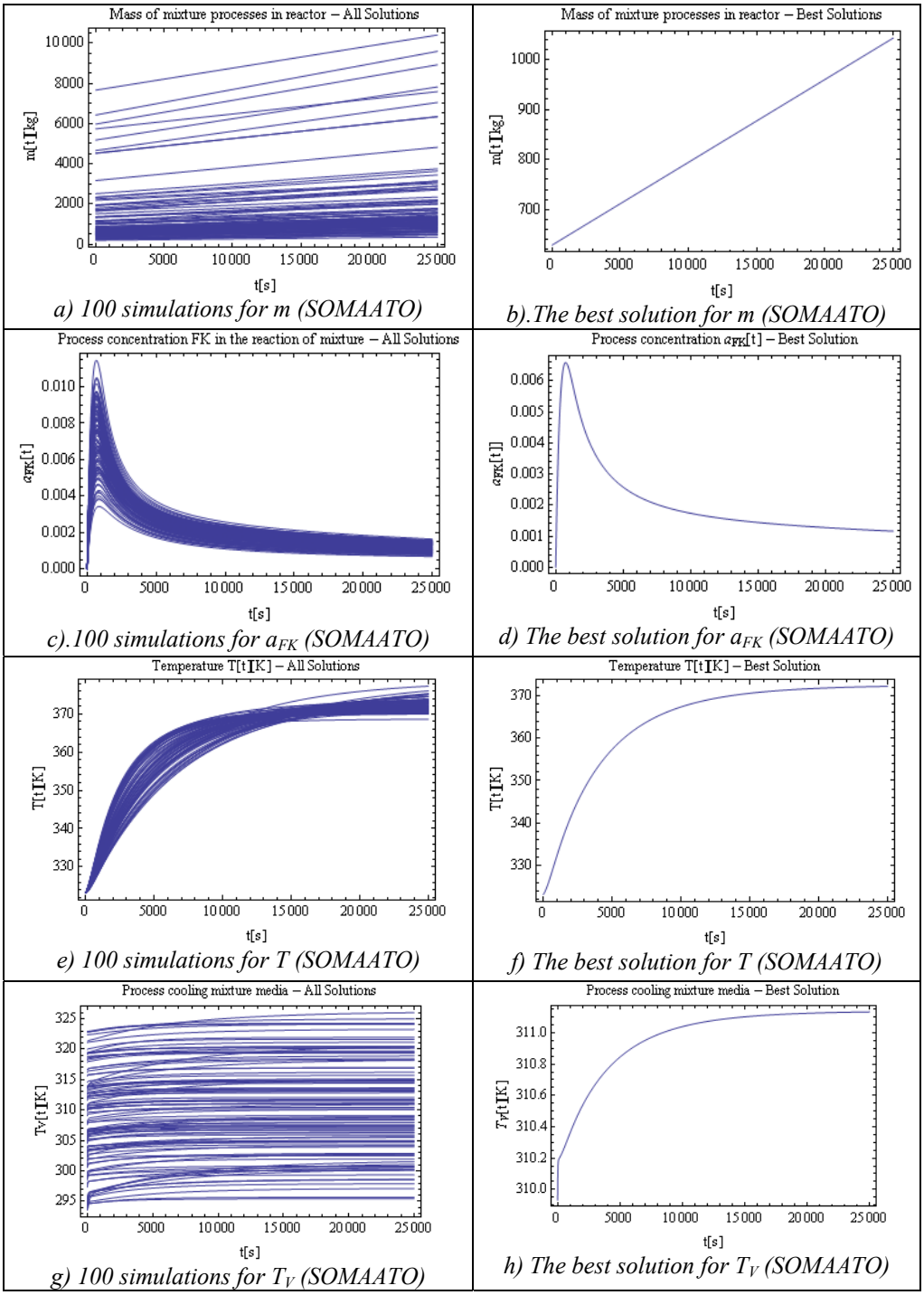
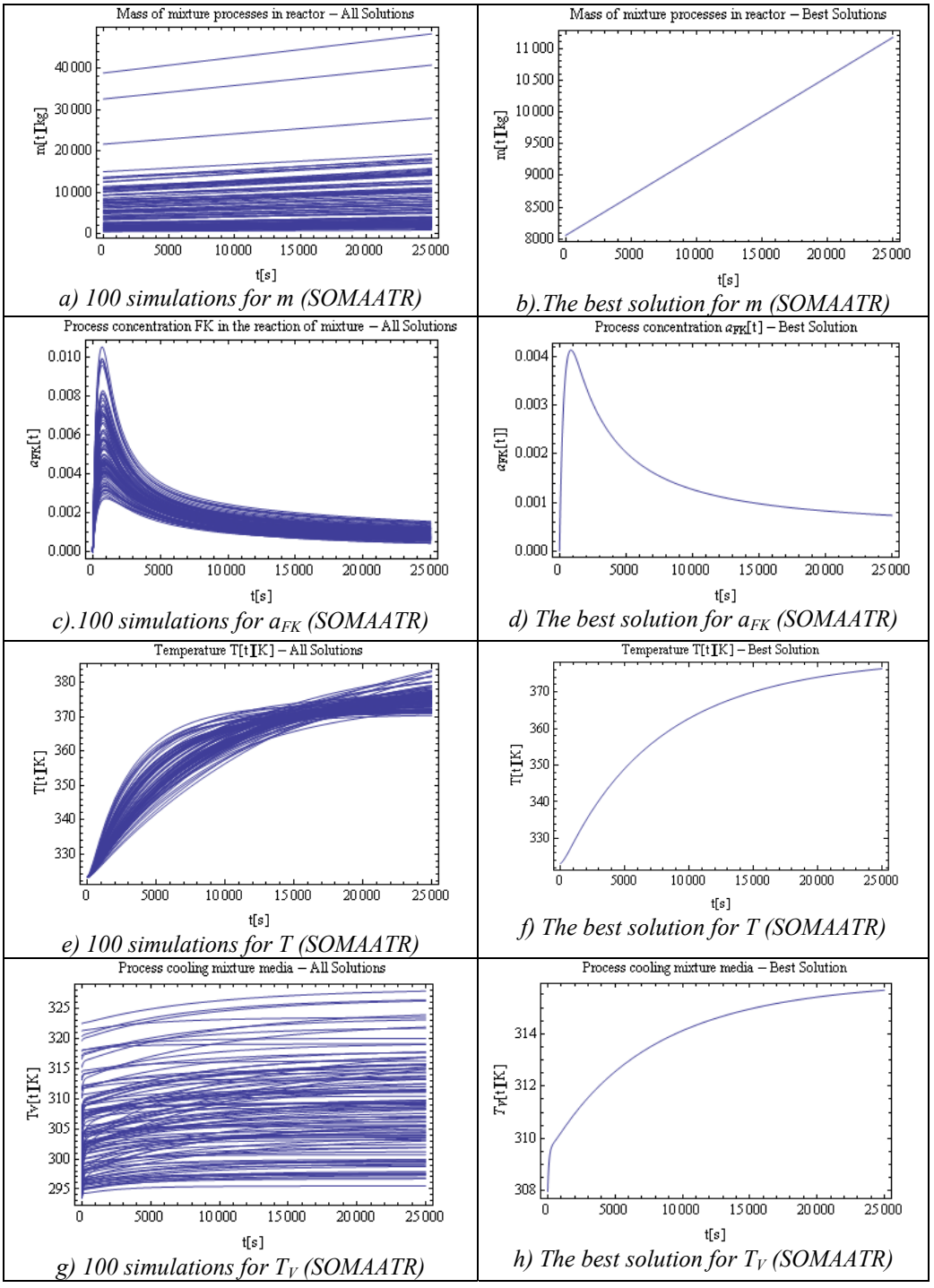


Fig. 20. Process parameters for 100 simulations of SOMA - version SOMAATO



a) 100 simulations for m (SOMAATR)

b).The best solution for m (SOMAATR)

c).100 simulations for a_{FK} (SOMAATR)

d) The best solution for a_{FK} (SOMAATR)

e) 100 simulations for T (SOMAATR)

f) The best solution for T (SOMAATR)

g) 100 simulations for T_V (SOMAATR)

h) The best solution for T_V (SOMAATR)

Fig. 21. Process parameters for 100 simulations of SOMA - version SOMAATR

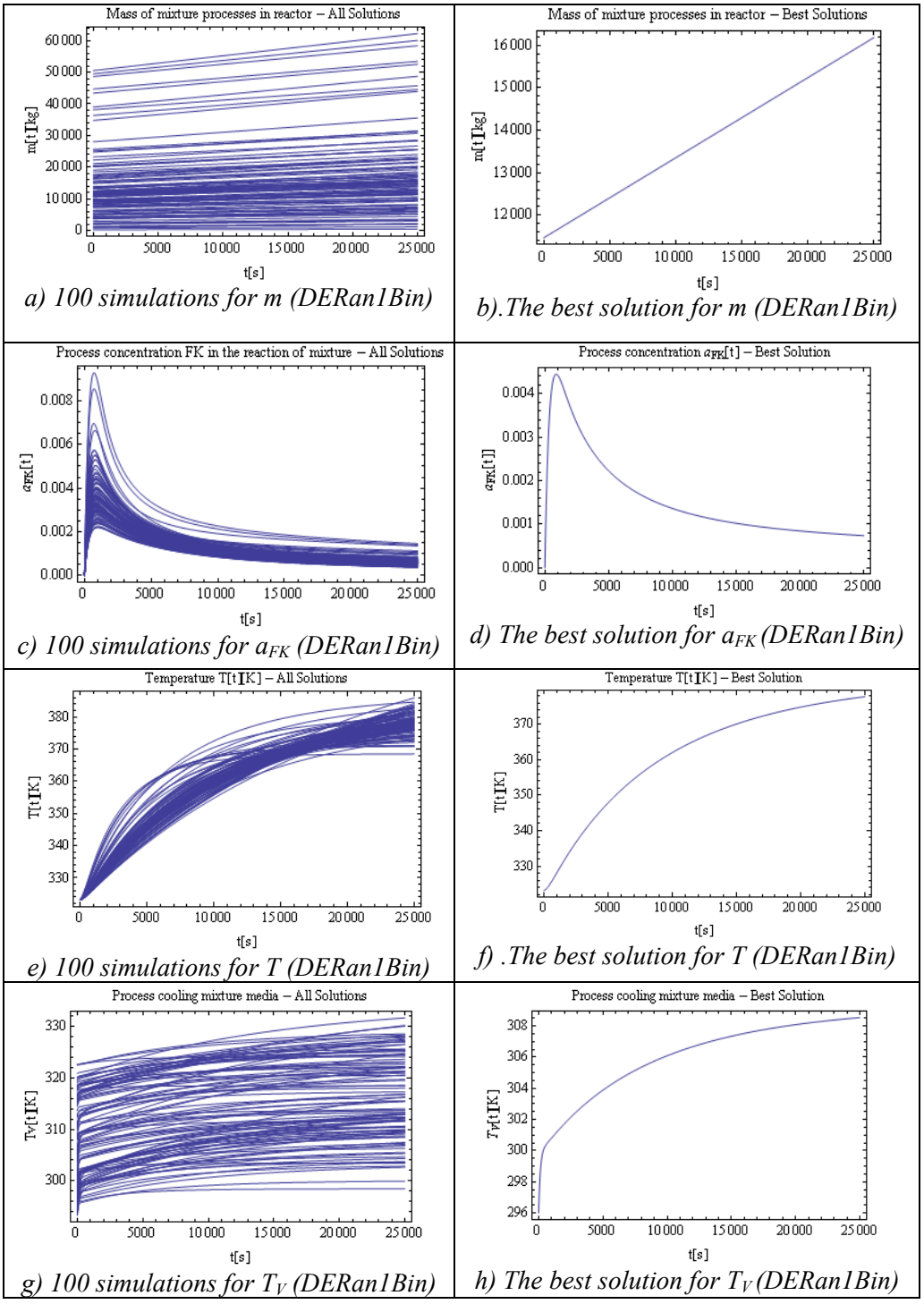


Fig. 22. Process parameters for 100 simulations of DE - version DERan1Bin

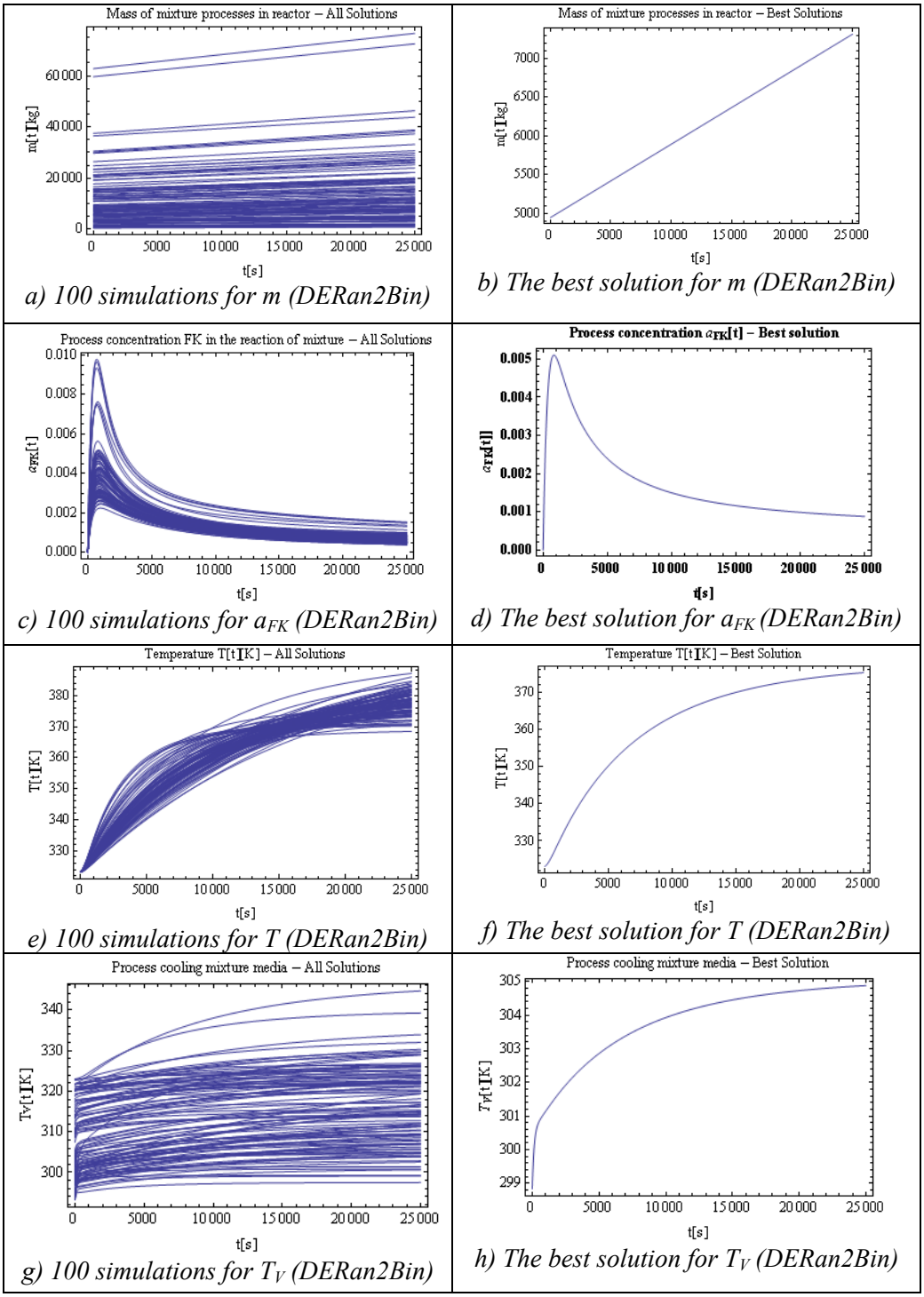


Fig. 23. Process parameters for 100 simulations of DE - version DERan2Bin

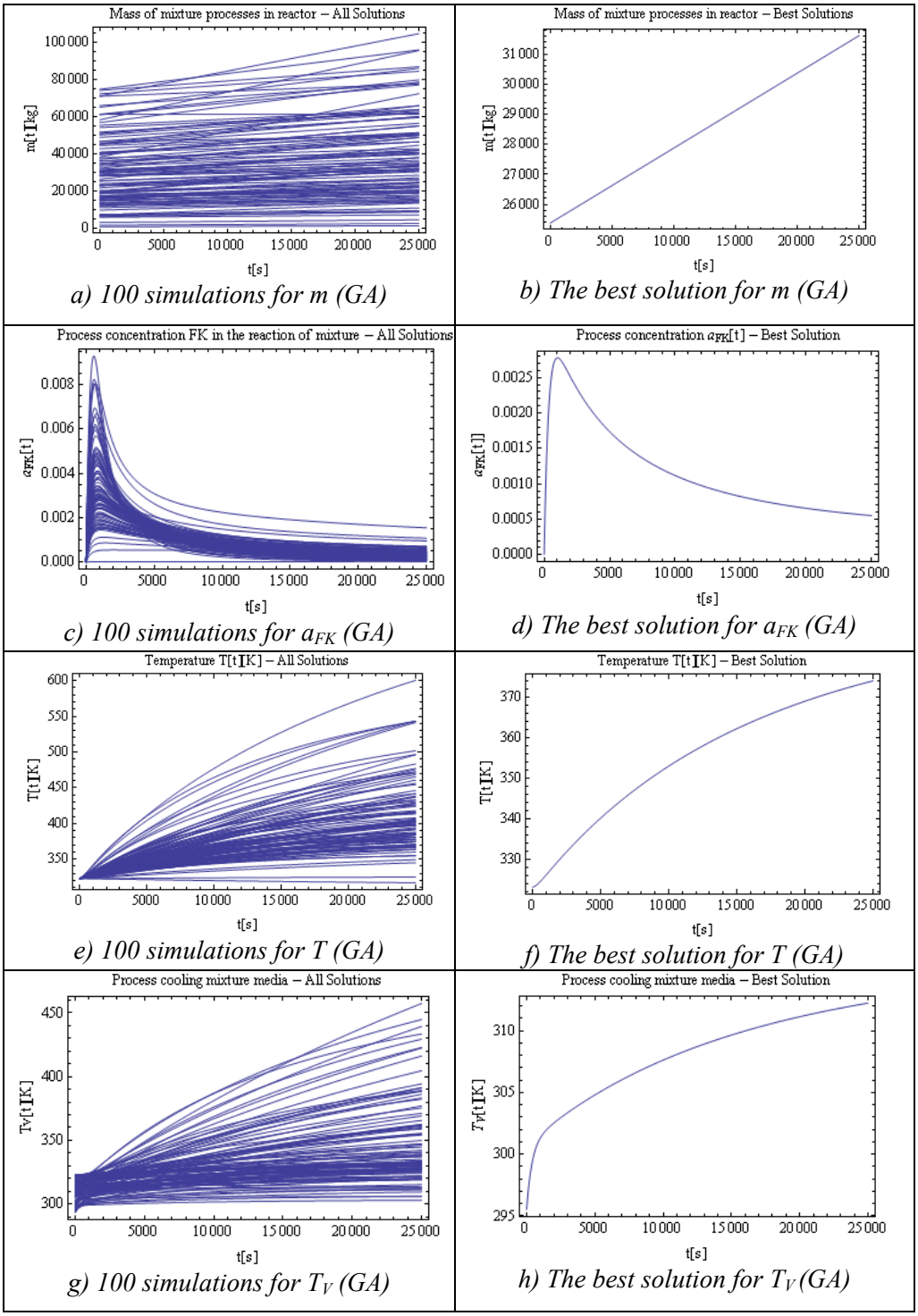


Fig. 24. Process parameters for 100 simulations of GA

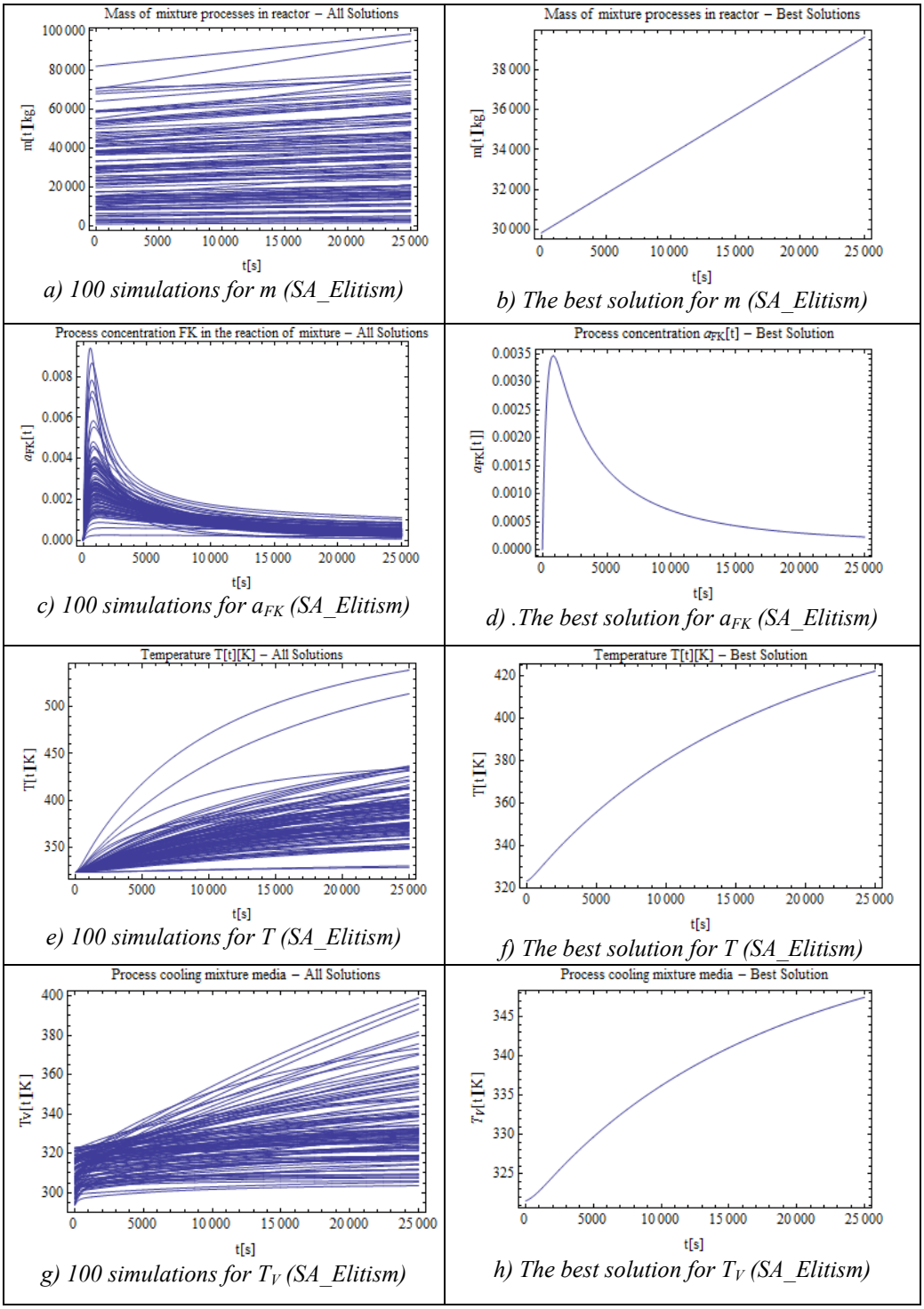


Fig. 25. Process parameters for 100 simulations of SA – version SA_Elitism

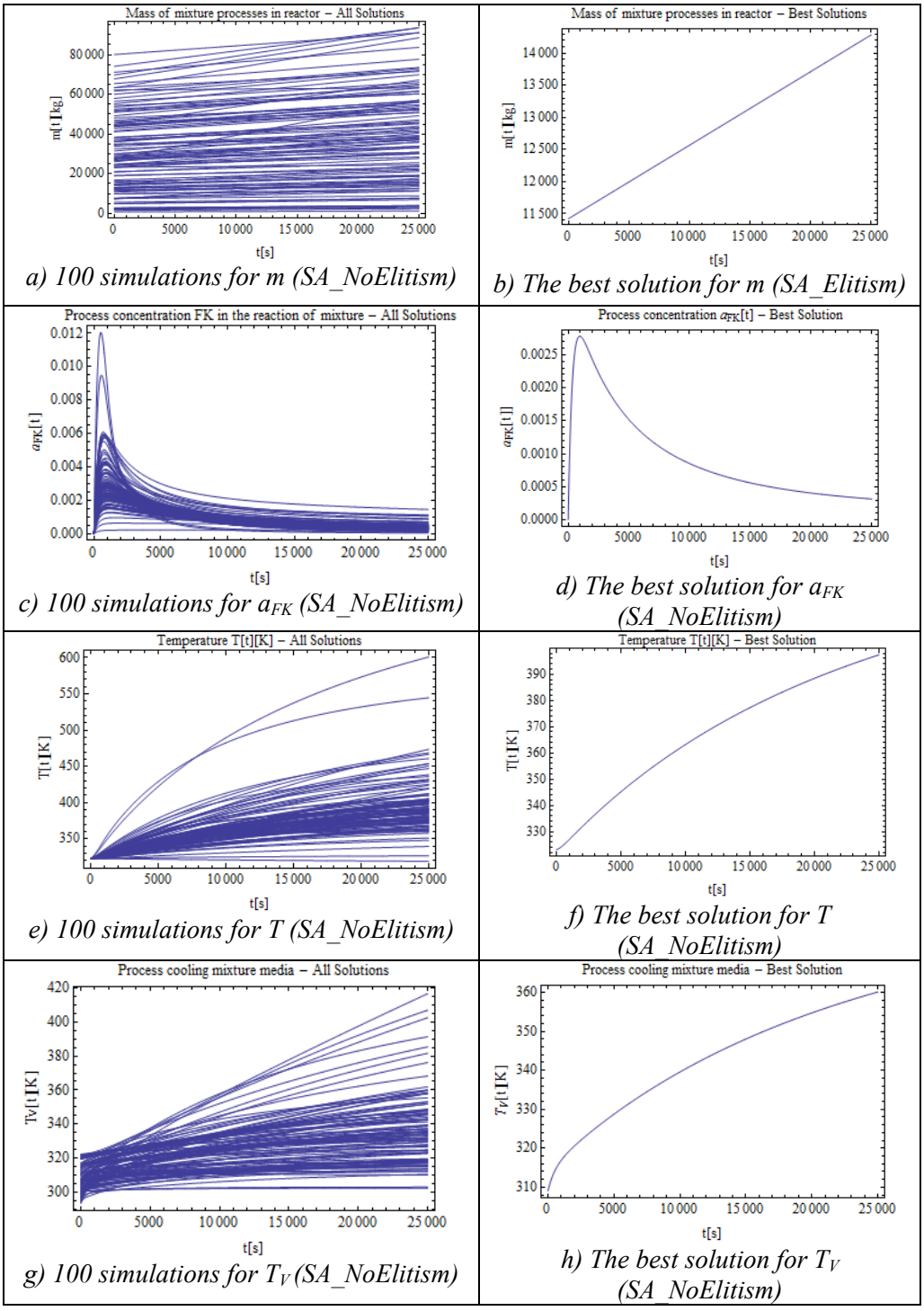


Fig. 26. Process parameters for 100 simulations of SA – version SA_NoElitism

5.3.3.5 Discussion to the results optimization

This project of thesis has presented a systematic procedure to derive a solution model for operation of a dynamic chemical reactor process. The results produced by the optimizations depend not only on the problem being solved but also on the way how to define a given function. All simulations were repeated 100 times for each EA with the same initial conditions for each simulation. In total, 2800 (7 algorithms×4 case studies×100 repeated experiments) independent simulations were conducted of real-time optimization of Batch reactor on Power Mac G5 Quad 2.5 GHz with software Grid Mathematica®.

The differences between four methods SOMA, DE, GA and SA are best seen in Tab.6, Tab. 7 and Tab.8. The first part shows the parameters of batch reactor designed by an expert , and the second part shows the parameters obtained through static optimization.

Calculation was 100 times repeated and the best, worst and average result (individual) was recorded from the last population in each simulation. All one hundred triplets (best, worst, average) were used to create Fig. 18 and Fig.19.

Four algorithms (SOMA, DE, GA, SA) have been applied 100 times in order to find the optimum of process parameters and the reactor geometry. The primary aim of this comparative study is not to show which algorithm is better or worse. But in this investigation, the results from the outputs of all simulations are depicted in Fig. 22-26 show that evolution SOMA represents the best solution from actual simulation more than DE, GA and SA. Based on data from all simulations, four comparisons can be done. From parameter variation of view, the estimated parameters depicted in Fig.18 & Fig.19 show that four algorithms are comparable in performance (with small deviations).

From the graphs, it is evident that the courses of SOMA algorithm are more densities in a thin spectra and not far from the start of mass axis (see Fig. 20a). Only few values drifting out of the spectra. From these results we may conclude, that SOMA has much better convergence than DE, GA, SA algorithm (see Fig.20 - Fig.26). Or for better overview of comparison between four algorithms, I have chosen processes temperature of reactionary mixture *T,* show in Fig. 27

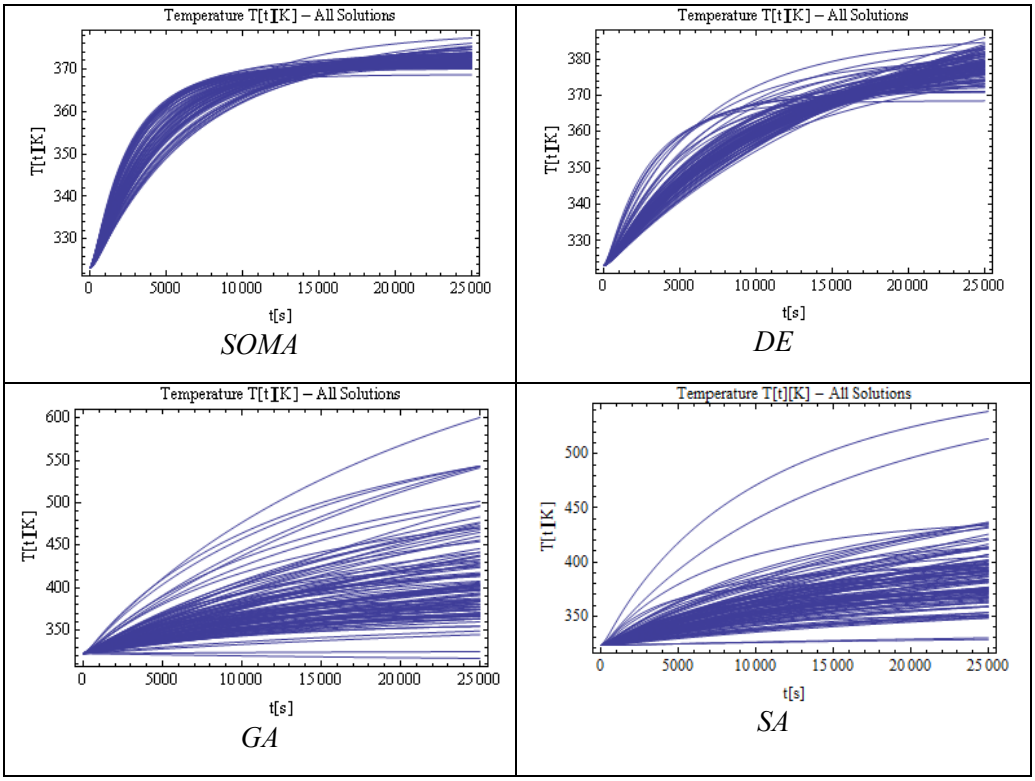


Fig. 27. 100 simulations for T

In Fig. 27 we can see the process parameters temperature *T* simulation by SOMA were stability more than other algorithms (concretely, in this experimental problem of Batch reactor).

From the obtained results, it is possible to say that all simulations give satisfactory results and thus **evolutionary algorithms are capable of solving this class of difficult problems and the quality of results does not depend only on the problem being solved but they are extremely sensitive on the proper definition of the cost function, selection of parameters setting of evolutionary algorithms.**

5.3.4 Optimization of Continuous stirred tank reactor

5.3.4.1 Mathematical problems

Consider a CSTR with the first order consecutive exothermic reaction according to the scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ and with a perfectly mixed cooling jacket. The model CSTR show in Fig. 28. Using the usual simplifications, the model of the CSTR is described by four nonlinear differential equations.

$$\frac{d\,c_A}{dt} = -\left(\frac{Q_r}{V_r} + k_1\right) c_A + \frac{Q_r}{V_r} c_{Ai} \tag{5.12}$$

$$\frac{dc_B}{dt} = -\left(\frac{Q_r}{V_r} + k_2\right) c_B + k_1 c_A + \frac{Q_r}{V_r} c_{Bi} \tag{5.13}$$

$$\frac{dT_r}{dt} = \frac{h_r}{(\rho c_p)_r} + \frac{Q_r}{V_r}(T_{ri} - T_r) + \frac{A_h U}{V_r(\rho c_p)_r}(T_c - T_r) \tag{5.14}$$

$$\frac{dT_c}{dt} = \frac{Q_c}{V_c}(T_{ci} - T_c) + \frac{A_h U}{V_c(\rho c_p)_c}(T_r - T_c) \tag{5.15}$$

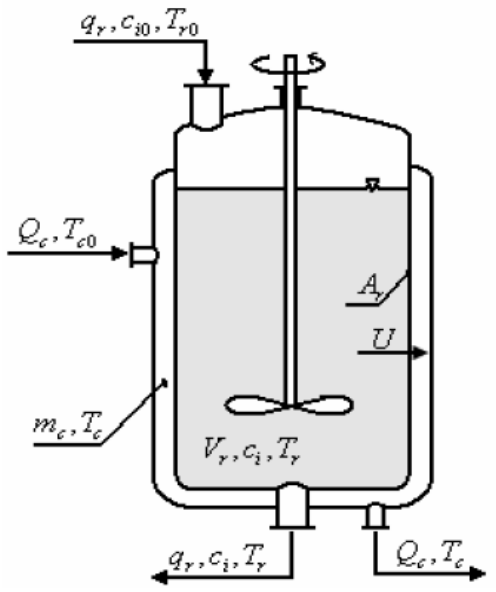


Fig. 28. Continuous Stirred Tank reactor

with initial conditions $c_A(0) = c_A^s$, $c_B(0) = c_B^s$, $T_r(0) = T_r^s$ and $T_c(0) = T_c^s$. Here, t is the time, c are concentrations, T are temperatures, V are volumes, ρ are densities, c_p are specific heat capacities, Q are volumetric flow rates, A_r is the heat exchange surface area and U is the heat transfer coefficient. The subscripts are denoted (.)r for the reactant mixture, (.)c for the coolant, (.)i for feed (inlet) values and the superscript (.)s for steady-state values. The reaction rates and the reaction heat are expressed as

$$k_j = k_{0j} \exp\left(\frac{-E_j}{RT_r}\right), \; j = 1, 2 \tag{5.16}$$

$$h_r = h_1 k_1 c_A + h_2 k_2 c_B \tag{5.17}$$

where k_0 are pre-exponential factors, E are activation energies and h are reaction entalpies. The values of all parameters, feed values and steady-state values are given in

Tab. 16 Parameters, inlet values and initial conditions

$V_r = 1.2$ m^3	$Q_r = 0.08$ m^{3}min^{-1}
$V_c = 0.64$ m^3	$Q_c^s = 0.03$ m^{3}min^{-1}
$\rho_r = 985$ kg m^{-3}	$c_{pr} = 4.05$ kJ kg^{-1}K^{-1}
$\rho_c = 998$ kg m^{-3}	$c_{pc} = 4.18$ kJ kg^{-1}K^{-1}
$A_r = 5.5$ m^2	$U = 43.5$ kJ m^{-2}min^{-1}K^{-1}
$k_{10} = 5.616 \cdot 10^{16}$ min^{-1}	$E_1/R = 13477$ K
$k_{20} = 1.128 \cdot 10^{18}$ min^{-1}	$E_2/R = 15290$ K
$h_1 = 4.8 \cdot 10^4$ kJ kmol^{-1}	$h_2 = 2.2 \cdot 10^4$ kJ kmol^{-1}
$c_{Ai} = 2.85$ kmol m^{-3}	$c_{Bi} = 0$ kmol m^{-3}
$T_{ri} = 323$ K	$T_{ci} = 293$ K
$c_A^s = 0.1649$ kmol m^{-3}	$c_B^s = 0.9435$ kmol m^{-3}
$T_r^s = 350.19$ K	$T_c^s = 330.55$ K

5.3.5 *Static optimization reactor*

In this model of CSTR the parameters were optimized include: the parameters of volumetric flow rates of the reactant mixture and the coolant Q_r, Q_c, the parameter of concentration for feed values c_{Ai} and temperature reactant mixture and colant T_{ri}, T_{ci}.

Tab. 17. Parameters of reactor, "yellow" was optimized

$V_r \rightarrow \text{Meter}^3$	$V_c \rightarrow \text{Meter}^3$	$\rho_r \rightarrow \frac{\text{Kilogram}}{\text{Meter}^3}$	$\rho_c \rightarrow \frac{\text{Kilogram}}{\text{Meter}^3}$
$A_r \rightarrow \text{Meter}^2$	$Q_r \rightarrow \frac{\text{Meter}^3}{\text{min}}$	$Q_c \rightarrow \frac{\text{Meter}^3}{\text{min}}$	$c_{pr} \rightarrow \frac{\text{KiloJoule}}{\text{KilogramKelvin}}$
$c_{pc} \rightarrow \frac{\text{KiloJoule}}{\text{Kilogram Kelvin}}$	$U \rightarrow \frac{\text{KiloJoule}}{\text{Meter}^2 \text{ min Kelvin}}$	$\frac{E_1}{R} \rightarrow \text{Kelvin}$	$\frac{E_2}{R} \rightarrow \text{Kelvin}$
$h_1 \rightarrow \frac{\text{KiloJoule}}{\text{KiloMole}}$	$h_2 \rightarrow \frac{\text{KiloJoule}}{\text{KiloMole}}$	$k_{10} \rightarrow \frac{1}{\text{min}}$	$k_{20} \rightarrow \frac{1}{\text{min}}$
$c_{Ai} \rightarrow \frac{\text{KiloMole}}{\text{Meter}^3}$	$c_{Bi} \rightarrow \frac{\text{KiloMole}}{\text{Meter}^3}$	$T_{ri} \rightarrow \text{Kelvin}$	$T_{ci} \rightarrow \text{Kelvin}$
$c_A^s \rightarrow \frac{\text{KiloMole}}{\text{Meter}^3}$	$c_B^s \rightarrow \frac{\text{KiloMole}}{\text{Meter}^3}$	$T_r^s \rightarrow \text{Kelvin}$	$T_c^s \rightarrow \text{Kelvin}$

5.3.5.1 The Cost Function (CF)

In this research, the objective was to minimize the area arising as a difference of the process between the observed and real selected time interval, which was the duration of a CSTRs cycle. With the inlet concentration $c_{Bi} = 0$ kmol m^{-3}, the cost function that was minimized is given in (5.17). In the cost function, we multiplied by (-1) in order to transfer from maximization into minimization.

$$f_{\cos t} = (-1) * \sum_{t=0}^{t} |c_B[t]| \tag{5.17}$$

5.3.5.2 Parameter settings

The control parameter settings for simulation by EAs of model CSTR have been found empirically and are given in Tab. 18 for SOMA. In this model o CSTR, I have changed number of migration from 50 to 10 and the parameters setting of algorithms DE, GA and SA are the same in the previous part of simulation for model of Batch reactor. Number of optimized reactor parameters and their range inside represents in Tab. 19.

Tab.18 SOMA parameter setting for simulation of CSTR model

	A
PathLength	3
Step	0.1
PRT	0.1
PopSize	20
Migrations	10
MinDiv	-1
Individual Length	6
CF Evaluations	5182

Tab.19 Optimized reactor parameters and their range inside which has been optimization done

Parameter	Range
Q_c [$m^3 min^{-1}$]	0.015 – 0.1
Q_r [$m^3 min^{-1}$]	0.05 – 0.012
c_{Ai} [kmol m^{-3}]	2 – 3.5
T_{ri} [K]	303 – 333
T_{ci} [K]	288-303

5.3.5.3 Experimental results

The best values of parameter setting are recorded in Tab. 20 & 21 of each algorithms SOMA, DE, GA, SA. Then, four algorithms have to been applied 100 times in order to find the optimum of process parameters and get data for statistical data processing. All important data has been visualized directly or/and processed for graphs demonstrating performance of this algorithms. Estimated parameters and their diversity (minimum, maximum and average) are depicted in Tab. 22 - Tab. 28. From those figures of parameter variation, it is visible that results from each of evolutionary algorithms are showed detail "optimal points". For the demonstration are graphically the best solutions shown in Fig. 29 & 30. On Fig. 31 - Fig. 34 are for example shown records of all 100 simulations of each algorithm.

Tab. 20. The best values of optimized parameters by SOMA, DE

Parameter	SOMAATO	SOMAATR	DERan1Bin	DERan2Bin
Q_c [m^3min^{-1}]	0.071157	0.0822537	0.0761633	0.0922708
Q_r [m^3min^{-1}]	0.119602	0.119802	0.119109	0.118459
c_{Ai} [kmol m^{-3}]	2.46777	2.26616	2.26559	3.46583
T_{ri} [K]	321.212	321.326	321.124	321.808
T_{ci} [K]	299.741	301.983	301.767	302.244

Tab. 21. The best values of optimized parameters by GA, SA

Parameter	GA	SA_Elitism	SA_NoElitism
Q_c [m^3min^{-1}]	0.0566459	0.0958446	0.0176245
Q_r [m^3min^{-1}]	0.107929	0.110968	0.111787
c_{Ai} [kmol m^{-3}]	2.22209	2.12066	2.38449
T_{ri} [K]	319.325	323.437	314.535
T_{ci} [K]	302.563	297.987	301.052

Tab.22 Estimated parameters of version SOMAATO

Parameter	Min	Avg	Max
Q_c [m^3min^{-1}]	0.0171178	0.0750863	0.0999769
Q_r [m^3min^{-1}]	0.103969	0.117765	0.119991
c_{Ai} [kmol m^{-3}]	2.01516	2.76918	3.48831
T_{ri} [K]	314.729	320.984	323.913
T_{ci} [K]	294.149	300.861	302.986

Tab.23 Estimated parameters of version SOMAATR

Parameter	Min	Avg	Max
Q_c [m^3min^{-1}]	0.0152446	0.0713548	0.0997426
Q_r [m^3min^{-1}]	0.101533	0.115791	0.119991
c_{Ai} [kmol m^{-3}]	2.00351	2.70686	3.4979
T_{ri} [K]	313.8	320.759	326.271
T_{ci} [K]	290.142	300.467	302.924

Tab.24 Estimated parameters of version DERan1Bin

Parameter	Min	Avg	Max
Q_c [m^3min^{-1}]	0.0165912	0.0771171	0.0997425
Q_r [m^3min^{-1}]	0.107223	0.117691	0.119999
c_{Ai} [kmol m^{-3}]	2.00871	2.70933	3.49065
T_{ri} [K]	314.373	321.107	325.252
T_{ci} [K]	291.929	300.735	302.959

Tab.25 Estimated parameters of version DERan2Bin

Parameter	Min	Avg	Max
Q_c [m^3min^{-1}]	0.0150441	0.076943	0.099324
Q_r [m^3min^{-1}]	0.111014	0.117478	0.119987
c_{Ai} [kmol m^{-3}]	2.00442	2.76267	3.4904
T_{ri} [K]	314.342	320.982	323.118
T_{ci} [K]	295.49	301.138	302.939

Tab.26 Estimated parameters of version GA

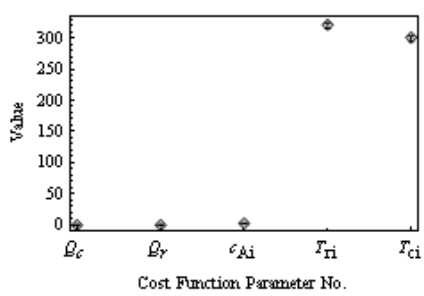
Parameter	Min	Avg	Max
Q_c [m^3min^{-1}]	0.0152769	0.0706135	0.0994583
Q_r [m^3min^{-1}]	0.105348	0.115416	0.119818
c_{Ai} [kmol m^{-3}]	2.00811	2.69678	3.49589
T_{ri} [K]	314.177	320.645	324.491
T_{ci} [K]	290.091	299.845	302.908

Tab.27 Estimated parameters of version SA_Elitism

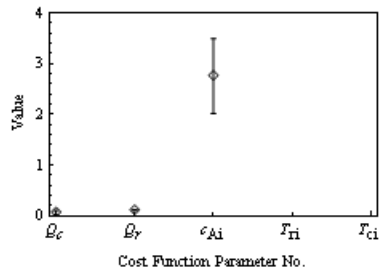
Parameter	Min	Avg	Max
Q_c [m^3min^{-1}]	0.0153787	0.0720453	0.0998463
Q_r [m^3min^{-1}]	0.108632	0.115819	0.119973
c_{Ai} [kmol m^{-3}]	2.00362	2.82362	3.47147
T_{ri} [K]	313.761	320.712	324.473
T_{ci} [K]	292.07	300.187	302.983

Tab.28 Estimated parameters of version SA_NoElitism

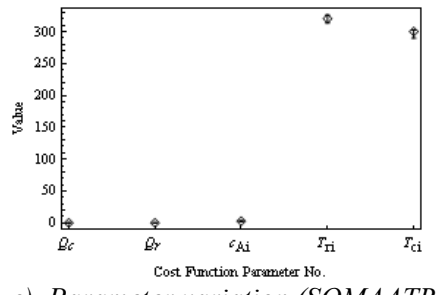
Parameter	Min	Avg	Max
Q_c [$m^3 min^{-1}$]	0.0162479	0.0733041	0.0998877
Q_r [$m^3 min^{-1}$]	0.103081	0.115918	0.119989
c_{Ai} [kmol m^{-3}]	2.0153	2.7703	3.48319
T_{ri} [K]	314.29	320.966	324.916
T_{ci} [K]	292.525	300.063	302.977



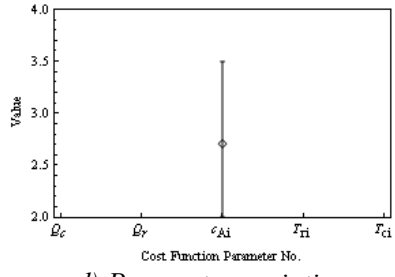
a) Parameter variation (SOMAATO)



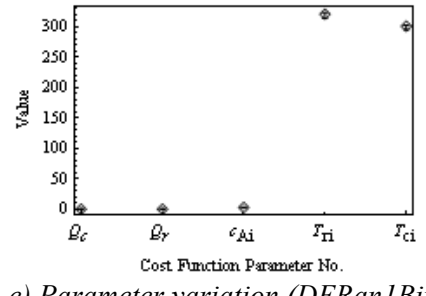
b) Parameter variation (SOMAATO)-detail



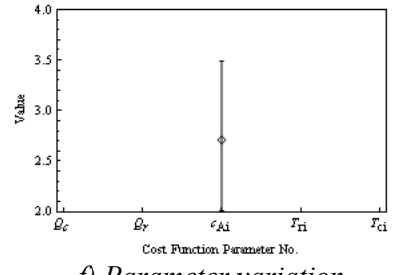
c) Parameter variation (SOMAATR)



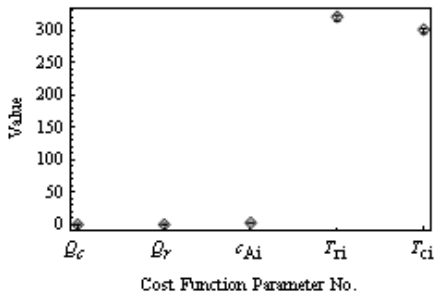
d) Parameter variation (SOMAATR)-detail



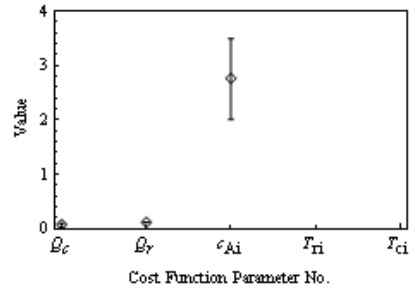
e) Parameter variation (DERan1Bin)



f) Parameter variation (DERan1Bin)-detail

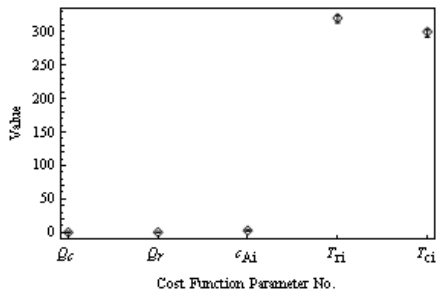


g) Parameter variation (DERan2Bin)

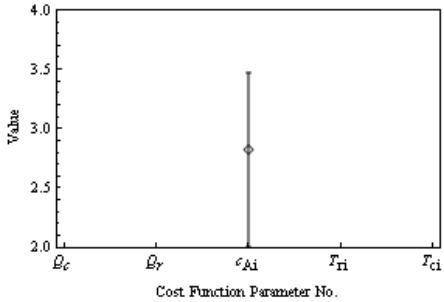


h) Parameter variation (DERan2Bin)-detail

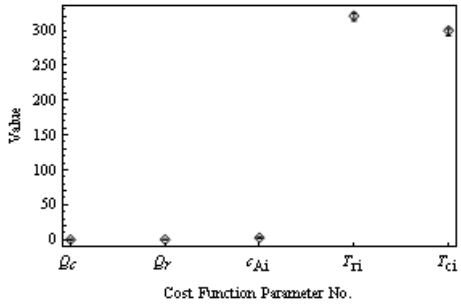
Fig. 29. Parameter variation of SOMA and DE for model CSTR



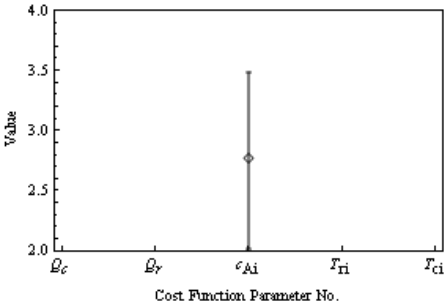
a) Parameter variation (SA_Elitism)



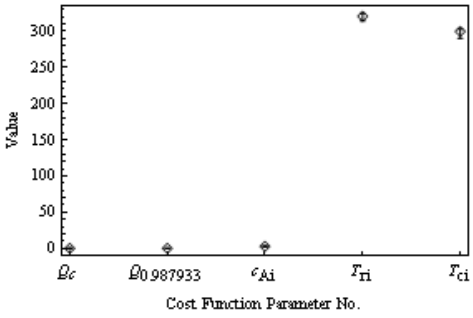
b) Parameter variation (SA_Elitism)-detail



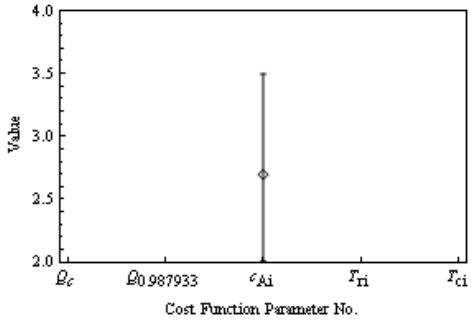
c) Parameter variation (SA_NoElitism)



d) Parameter variation (SA_NoElitism)

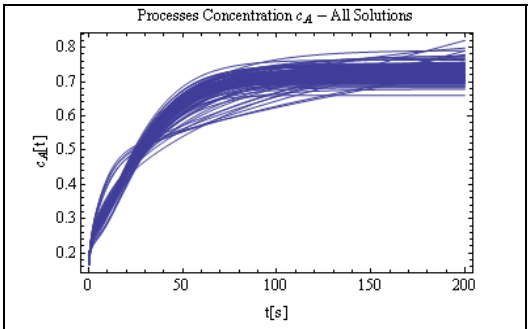


e) Parameter variation (GA)

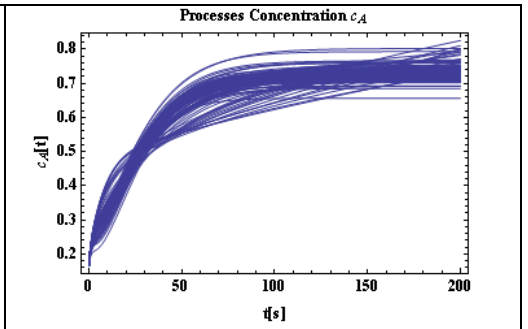


f). Parameter variation (GA)-detail

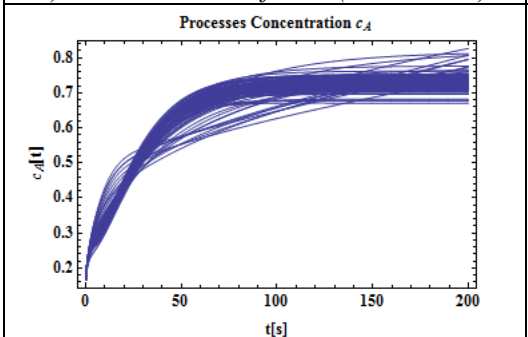
Fig. 30. Parameter variation of SA and GA for model CSTR



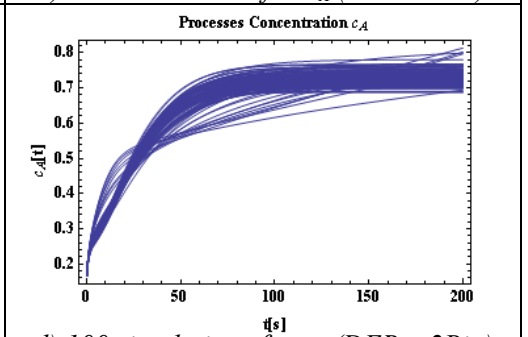
a) 100 simulations for c_A (SOMAATO)



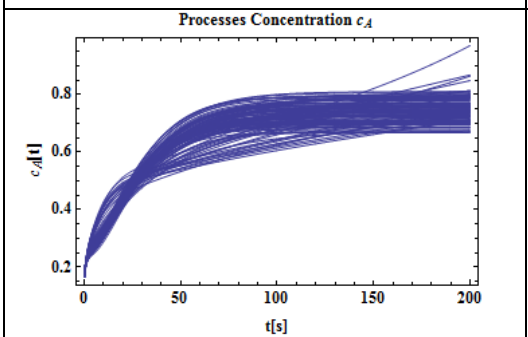
b) 100 simulations for c_A (SOMAATR)



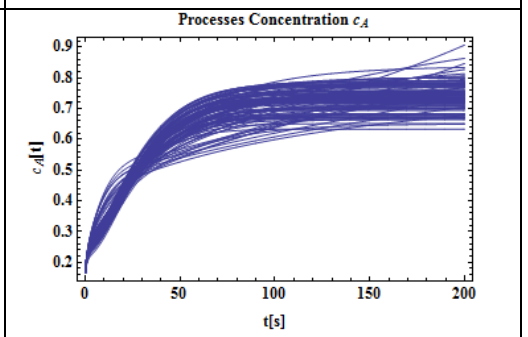
c) 100 simulations for c_A (DERan1Bin)



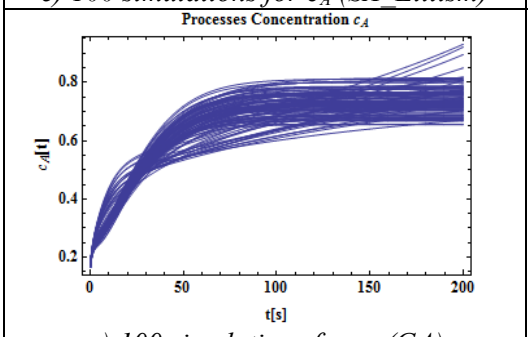
d) 100 simulations for c_A (DERan2Bin)



e) 100 simulations for c_A (SA_Elitism)

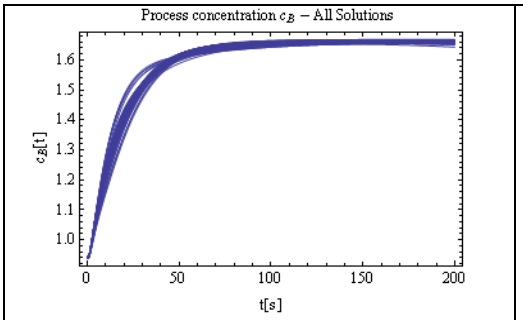


f) 100 simulations for c_A (SA_NoElitism)

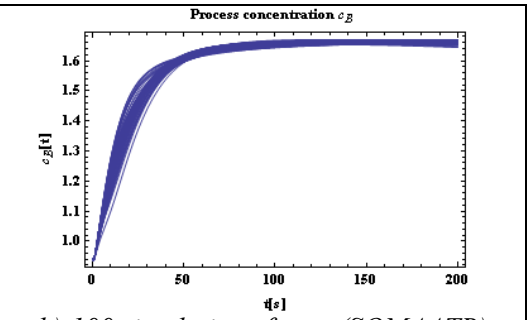


g) 100 simulations for c_A (GA)

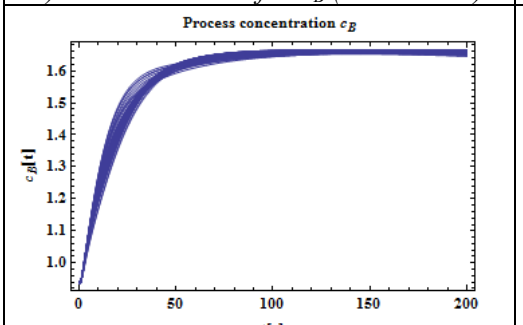
Fig. 31. Process parameters of c_A for 100 simulations of each algorithm



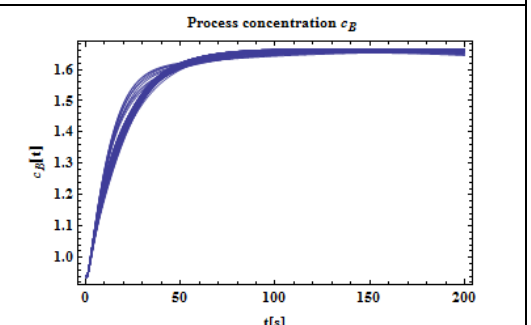
a) 100 simulations for c_B (SOMAATO)



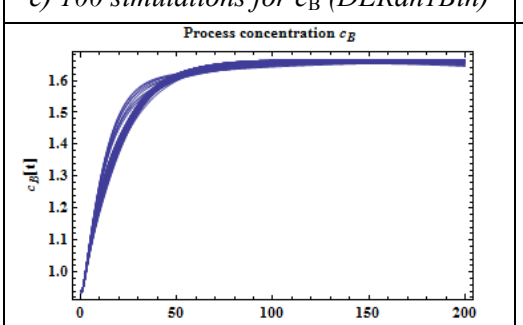
b) 100 simulations for c_B (SOMAATR)



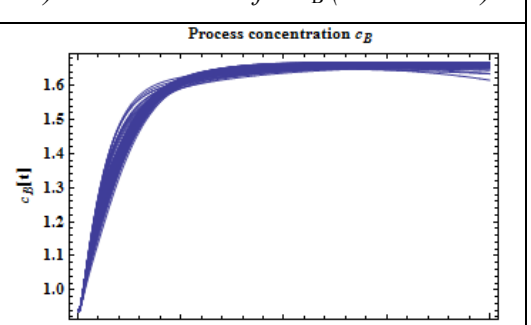
c) 100 simulations for c_B (DERan1Bin)



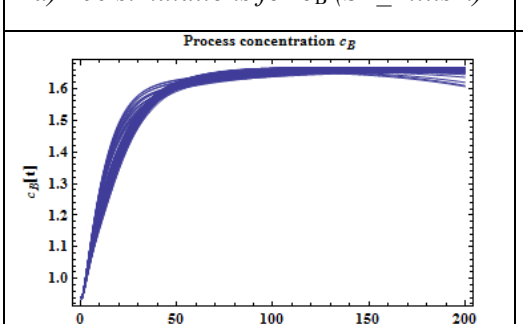
c) 100 simulations for c_B (DERan2Bin)



a) 100 simulations for c_B (SA_Elitism)

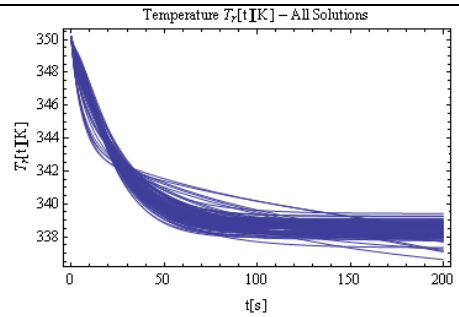


a) 100 simulations for c_B (SA_NoElitism)

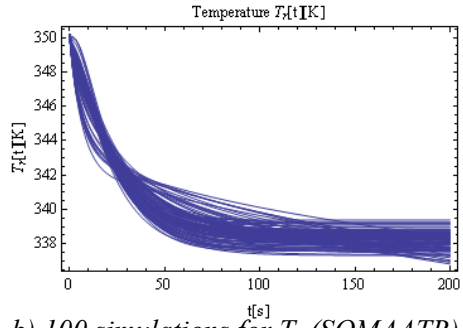


c) 100 simulations for c_B (GA)

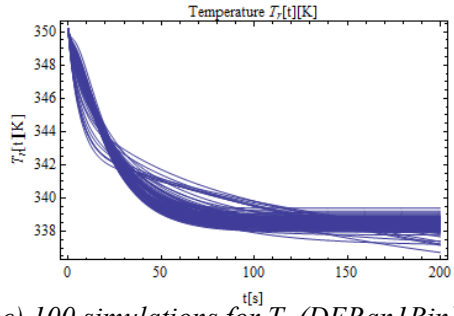
Fig. 32. Process parameters of c_B for 100 simulations of each algorithm



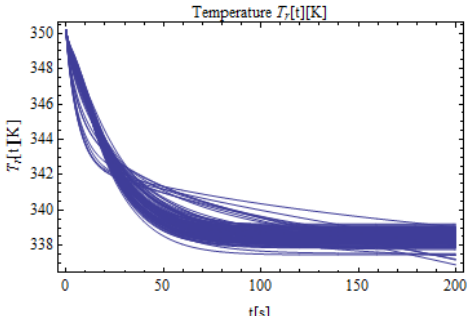
a) 100 simulations for T_r (SOMAATO)



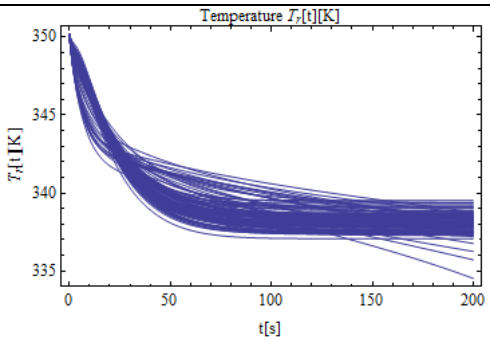
b) 100 simulations for T_r (SOMAATR)



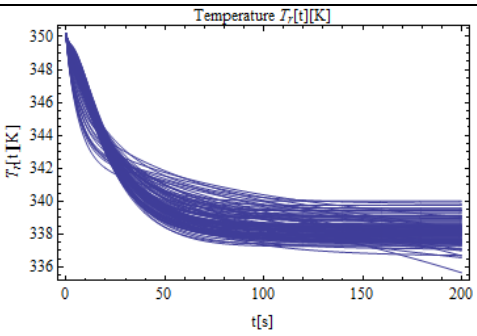
c) 100 simulations for T_r (DERan1Bin)



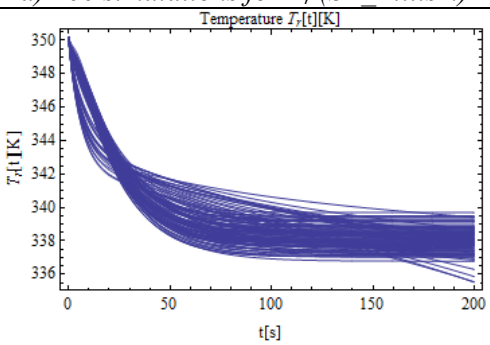
c) 100 simulations for T_r (DERan2Bin)



a) 100 simulations for T_r (SA_Elitism)

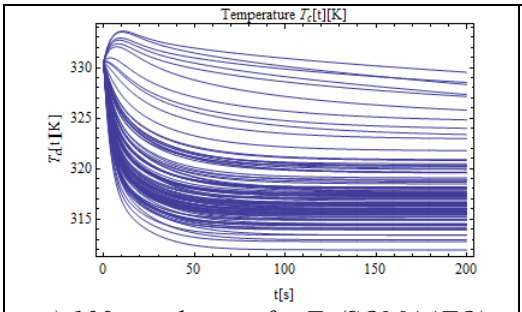


a) 100 simulations for T_r (SA_NoElitism)

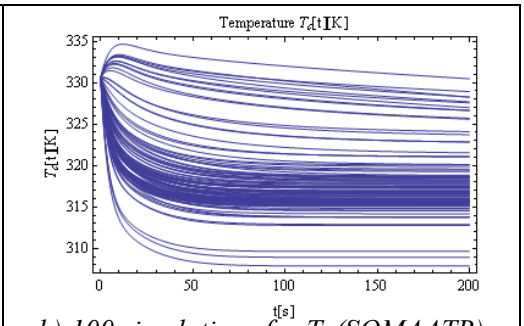


c) 100 simulations for T_r (GA)

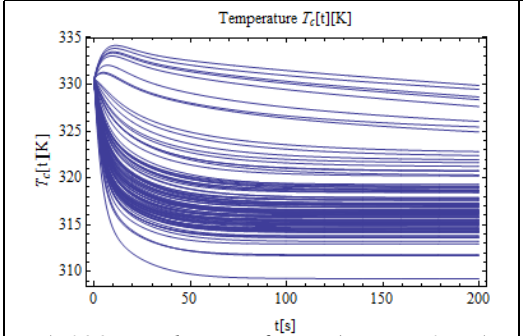
Fig. 33. Process parameters of T_r for 100 simulations of each algorithm



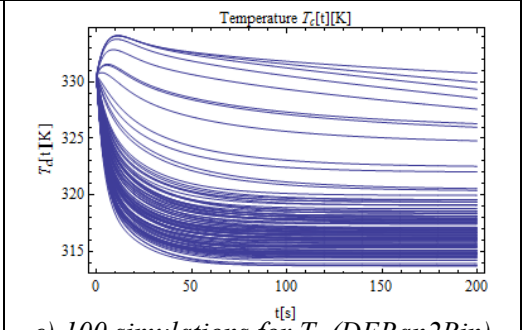
a) 100 simulations for T_c (SOMAATO)



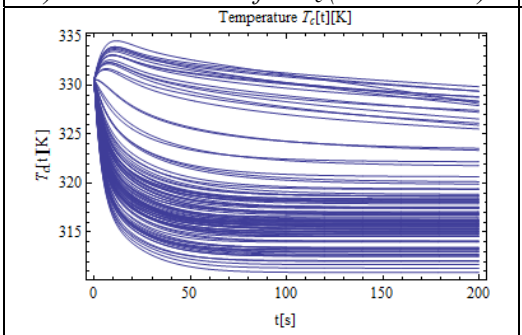
b) 100 simulations for T_c (SOMAATR)



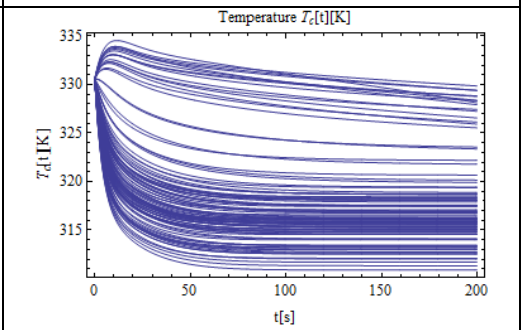
c) 100 simulations for T_c (DERan1Bin)



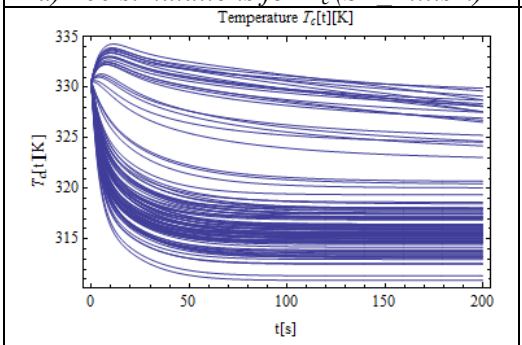
c) 100 simulations for T_c (DERan2Bin)



a) 100 simulations for T_c (SA_Elitism)



a) 100 simulations for T_c (SA_NoElitism)



c) 100 simulations for T_c (GA)

Fig. 34. Process parameters of T_c for 100 simulations of each algorithm

5.3.5.4 Discussion and conclusion

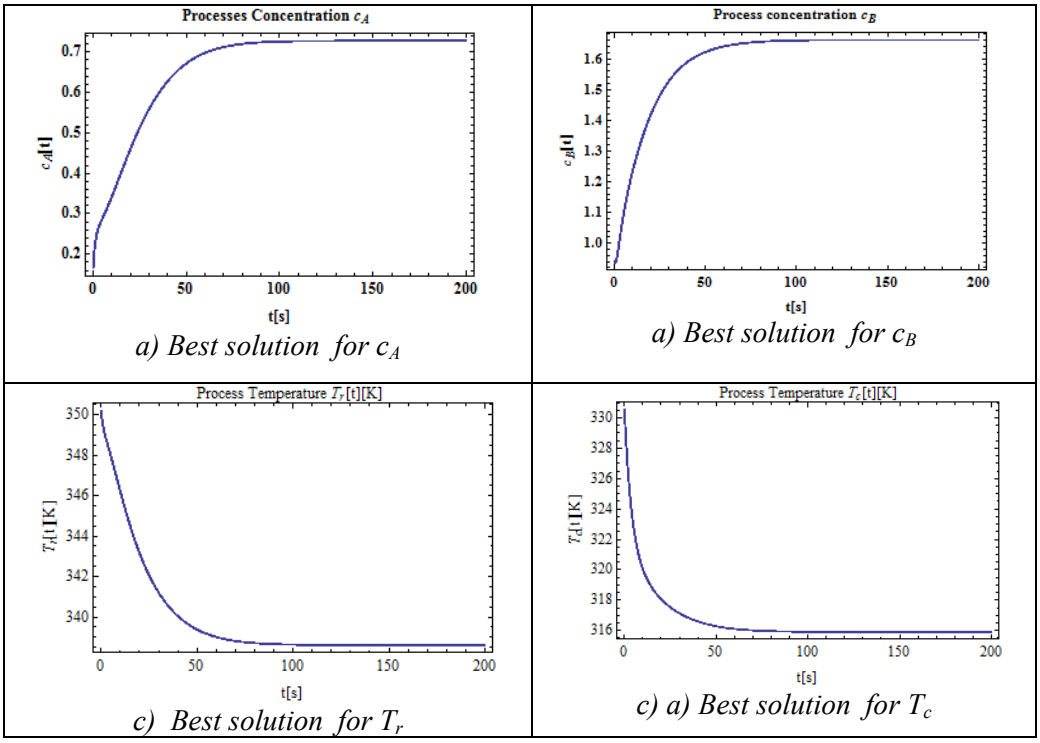
Just as in the case mentioned in the previous section for optimization of batch reactor, all simulations were repeated 100 times for each EA with the same principle simulation evolutionary algorithms. The parameters setting for EAs is the same in the case of optimization for bacth reactor, only I have changed number migrations of parameters setting of SOMA from 50 to 10 in order to get speedier simulation. The optimization by the cost function with concentration c_B show in (5.17) and time of each simulation is 200 seconds.

Calculation was 100 times repeated and the best, worst and average result (individual) was recorded from the last population in each simulation. All one hundred triplets (best, worst, average) were used to create Fig.29 & 30.

Compared with model of Batch, that the results from optimization on CSTR have obtained nearly resemblance. Estimated parameters and their diversity (minimum, maximum and average) are near approximately (see in Tab. 22-28). From the graphs of processes parameters for 100 simulations for c_A, c_B, T_r T_c (see Fig. 31-34) of each algorithm, it is very difficult to determine which algorithm is better. There are only small differences between them. On optimization of SOMA and DE, it is evident that the courses of algorithm are densities in a thin spectrum more than GA and SA. Alongside it, sometime few values drift out of the actual solution. But by the repetition of simulation was recorded the best result. On Fig. 35, the process of parameters by SOMA algorithm obtained best solution for the optimization.

Specially, there is difference between from both chosen model of chemical reactors (batch and CSTR). From investigation on optimization of process parameter of CSTR we can see, that four evolutionary algorithms (SOMA, DE, SA, GA) have obtained optimized results on very approximate value.

From these results we may conclude, that the quality and course of the evolutionary processes can be influenced by many factors, notably: setting parameters, definition of cost function, number of generations…. Moreover the results produced by the optimization process depends on the problem being solved, e.g. dynamical systems (mathematical and physical model).



a) Best solution for c_A

a) Best solution for c_B

c) Best solution for T_r

c) a) Best solution for T_c

Fig. 35. Best solution of SOMA

6 PREDICTIVE CONTROL

During the last decade, control scientists and experts have been thinking and given ideas in order to explore future directions of control theory and its applications. In addition, recent advances in computer technology, modern control techniques, and computational intelligence have opened a path for application of new generations of advanced process control algorithms (Takatsu et al., 1998; VanDoren, 1998).

Predictive control by mean evolutionary algorithms is very robust method, particular in system with many disturbing effects and failures. It's also a powerful tool in the search for optimal solutions to very complex problem in the field of control process. The basic idea is to find a set of action that lead to the principle optimization with required value. The block prediction procedure is shown in Fig. 36.

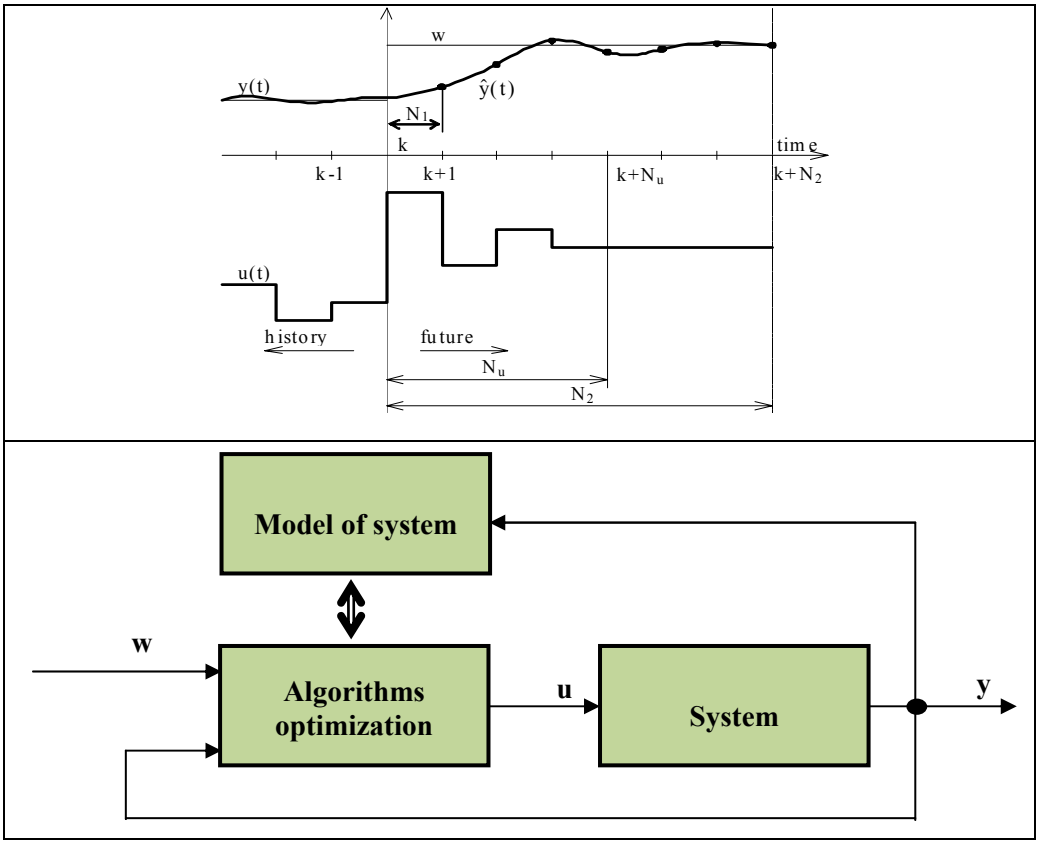


Fig. 36. Principle of predictive control by evolutionary algorithm

In block „Algorithms optimization“ are evolutionary algorithms, the predictive control is selected by minimising the commonly cost function *J*:

$$J(N_1, N_2, N_u) = \sum_{j=N_1}^{N_2} [y(k+j) - w(k+j)]^2 + \sum_{j=1}^{N_u} \lambda(j)[\Delta u(k+j-1)]^2 \qquad (6.1)$$

Here *y* is the output of system, *u* is actuating signal, *w* is the controlled value prediction, Δu is the control value change, *k* is the control step, N_1 is the lower and N_2 is the upper output prediction horizon, Nu is control horizon and λ is a weight sequence control of action.

Block "system" is a control process and block "model system" is used to predict its behaviour, it often represented in the appropriate algorithms of artificial intelligent, commonly artificial neural network.

Predictive control proceed that when change of required value running optimization algorithms in conjunction with model of system and minimising cost function (6.1) is found optimal action, which is for chosen system.

6.1 Principle simulation

In simulation of predictive control were used non-linear models, which were described in “problem design” of batch reactor and “mathematical problems” of CSTR. It was used such as block “system” and “model of system”. The principle simulation shown in Fig. 37.

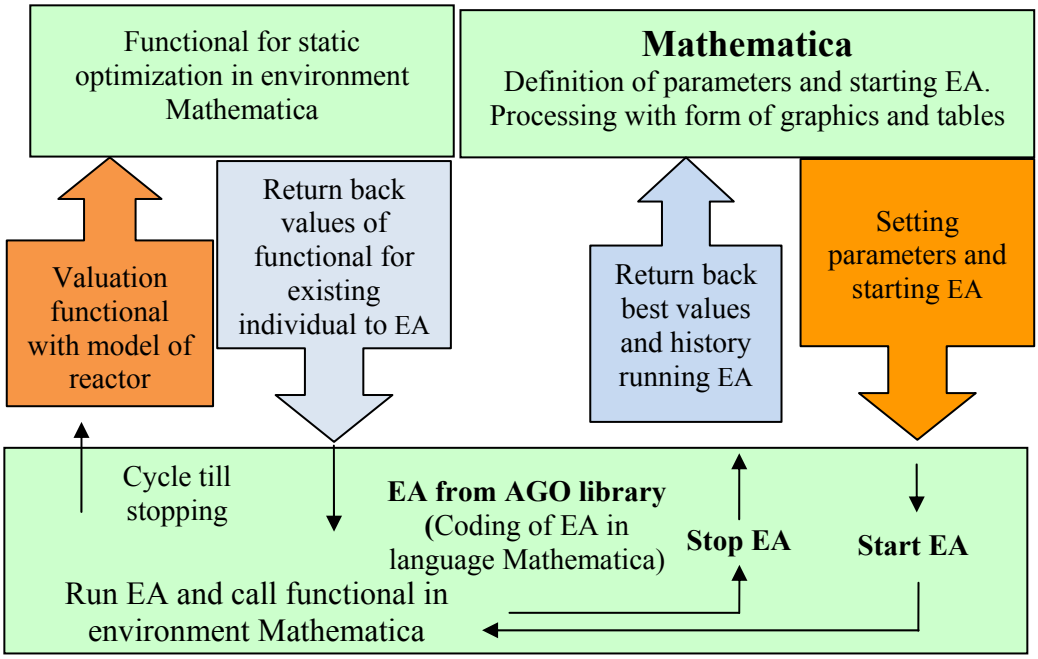


Fig. 37. Principle simulation

6.2 Optimization of CSTR value with prediction control

In this part of thesis, the temperature of CSTR reactor were chosen for prediction control. On this optimization the point was to minimize the area arising as a difference between the required and real temperature profile of the reaction mixture in a selected time interval, which was the duration of CSTR cycle. The cost functions that were minimized is given in (6.2) for T_c temperature and (6.3) for T_r.

$$f_{\cos t} = \sum_{t=0}^{t} \left| w_1 - T_r[t] \right| \tag{6.2}$$

$$f_{\cos t} = \sum_{t=0}^{t} \left| w_2 - T_c[t] \right| \tag{6.3}$$

Where w_1, w_2 are required values (control points)

For static optimization of CSTR value with prediction control we have added required value for simulation of temperature T_r and T_c belong following below Tab.29 & 30. The range inside of temperature T_r and T_c for predictive is <273.;380> [K].

Tab. 29 Range inside for predictive control of CSTR

Parameter	Range
T_r [K]	273 – 380
T_c [K]	273 – 380

Tab. 30. Parameters setting for predictive control of CSTR

Time simulation[s]	***Required value w_1 for T_r [K]***	***Required value w_2 for T_c [K]***
0 - 80	360	340
80 - 150	340	320
150 - 200	320	300
200 - 300	370	370

Simulations were conducted so that the first minimising cost function using the prediction horizon is found within the optimal action and intervention that was held for the control horizon. After that was calculated new intervention and has been applied during control horizon etc. till to do filling of reactor. For the CSTR reactor was selected: $N_1 = 1$, N_2 =300 a N_u = till to change.

6.3 Results of predictive control

On investigation of predictive control chemical reactor CSTR, I have chosen one basic version of each algorithm to optimize process parameters reactor. Concretely: version SOMAATO for SOMA; version DERan1Bin for

DE; version SA Elitism for SA. The evolutionary algorithms have been applied 100 times and the evolutionary processes of four algorithms show in follow graphs from Fig. 38 - 41.

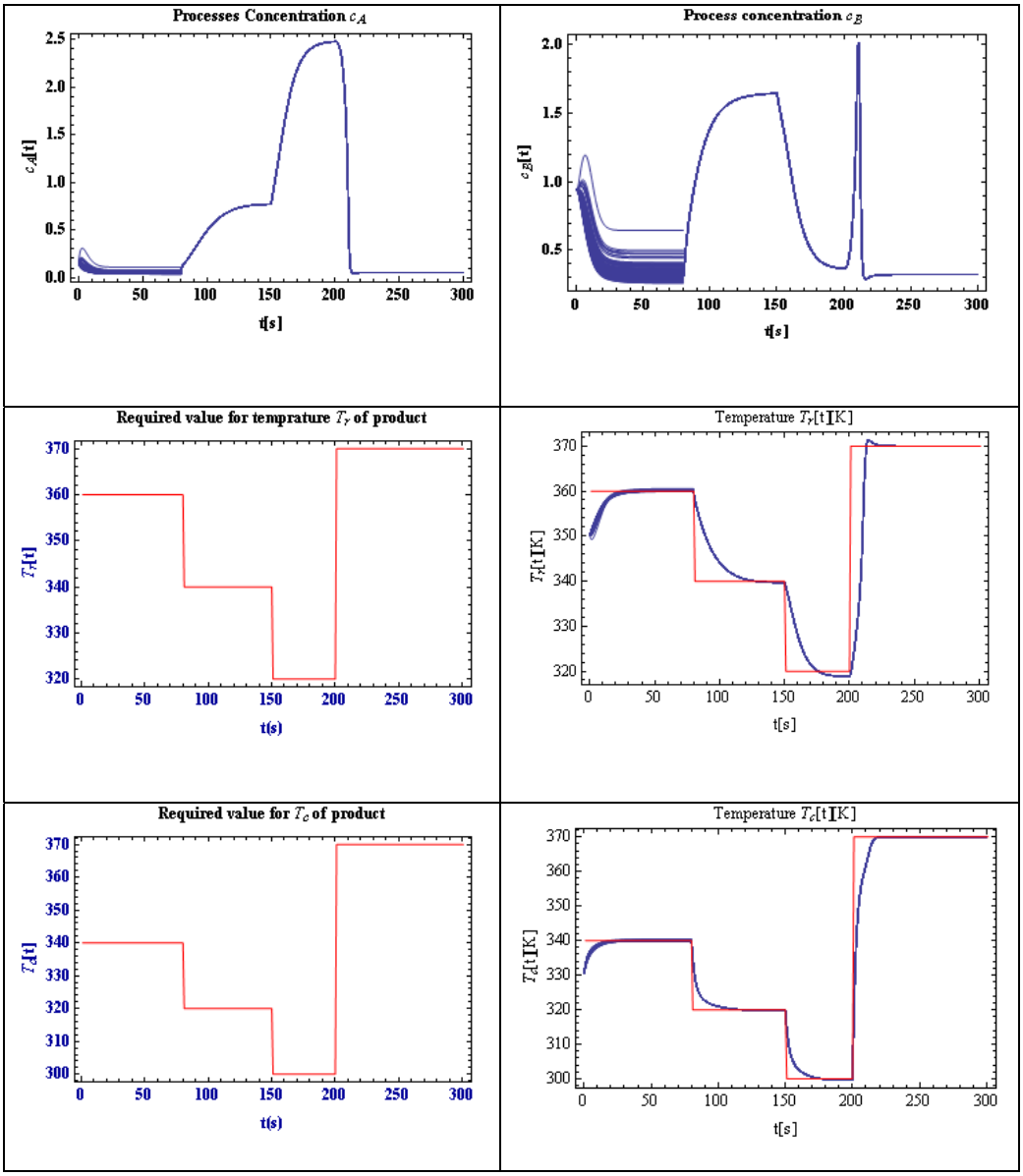


Fig. 38. Predictive control temperatures T_r and T_c of CSTR by SOMAATO, "red" was required value

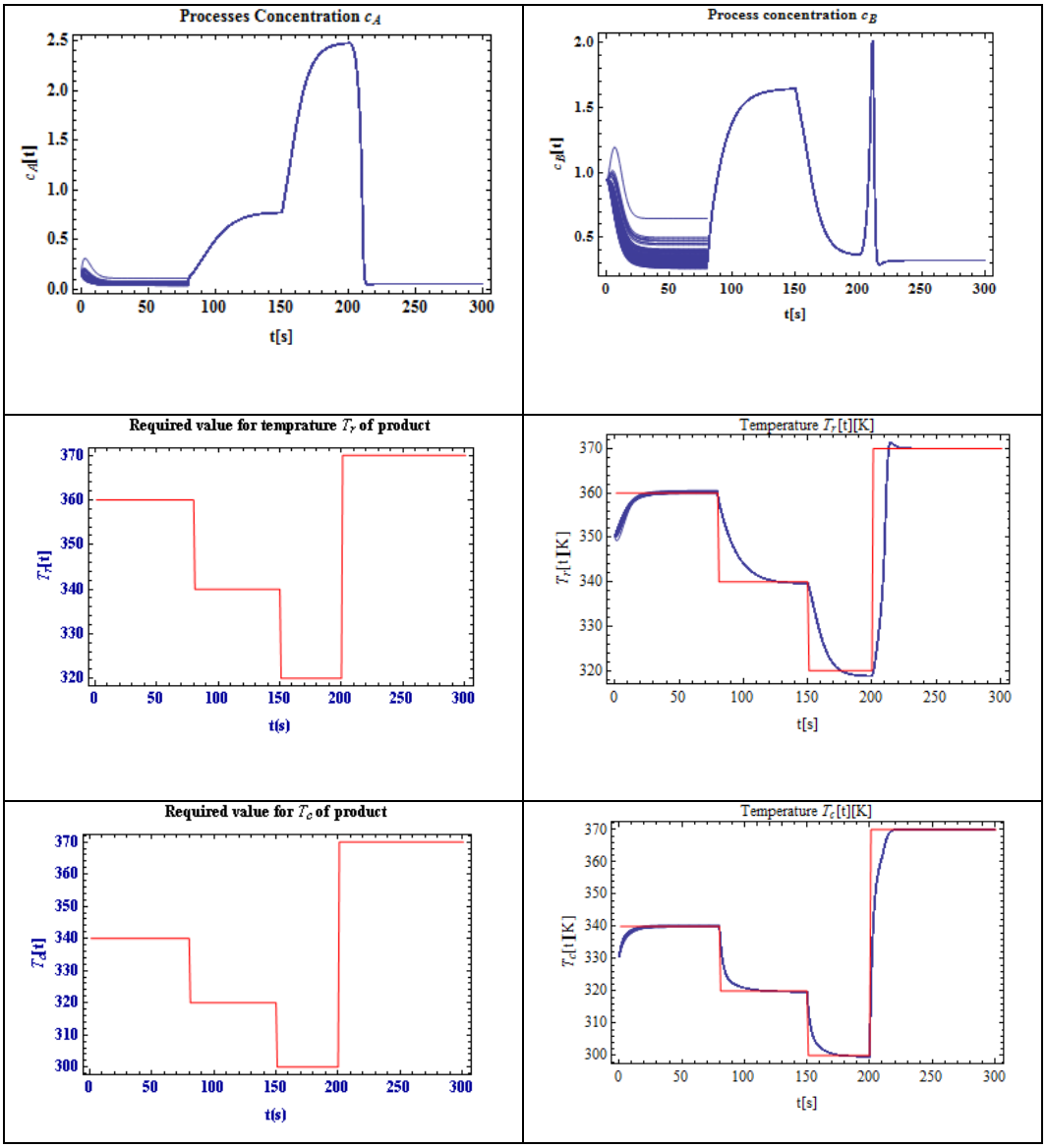


Fig. 39. Predictive control temperatures T_r and T_c of CSTR by DERan1Bin, "red" was required value

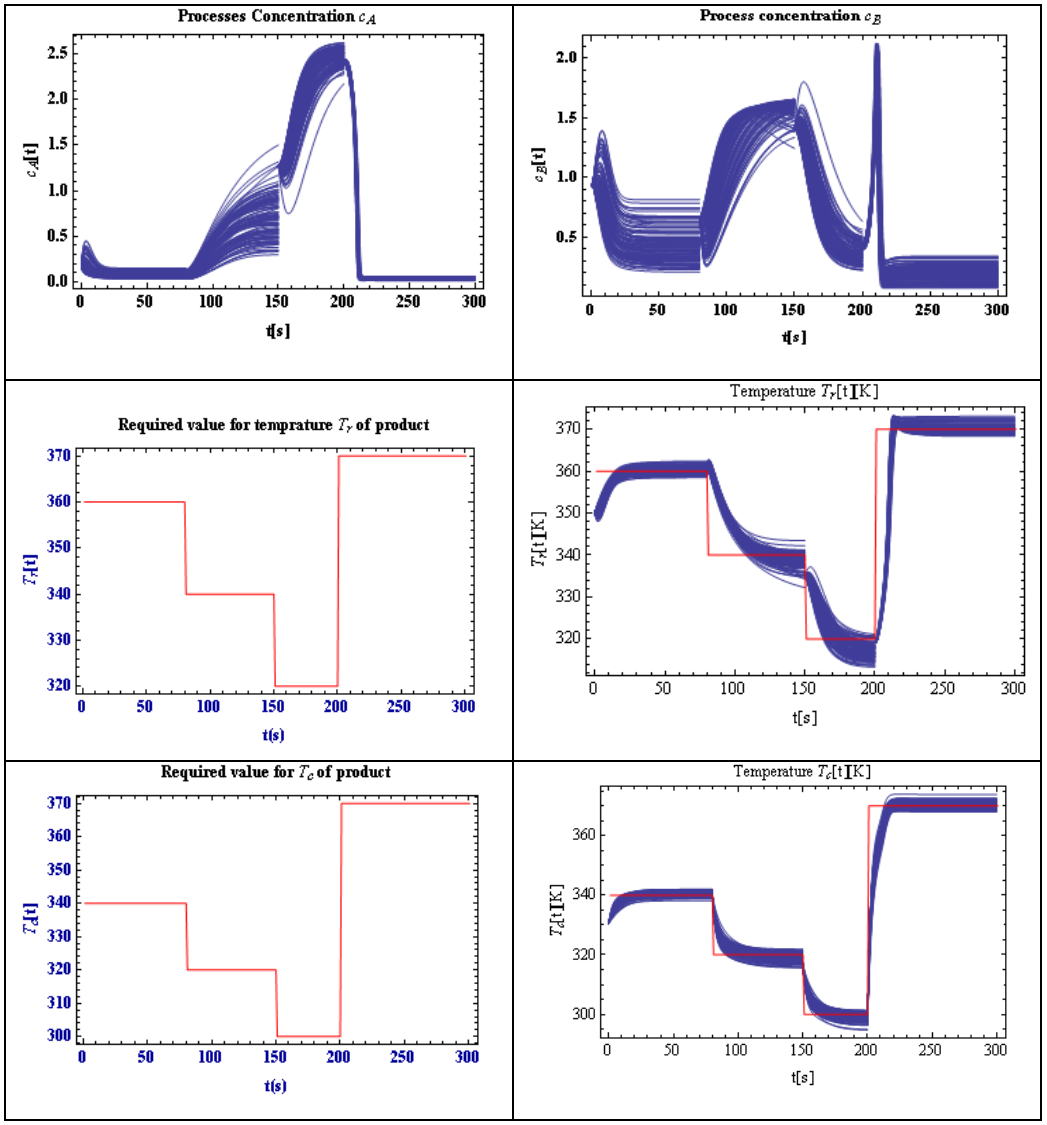
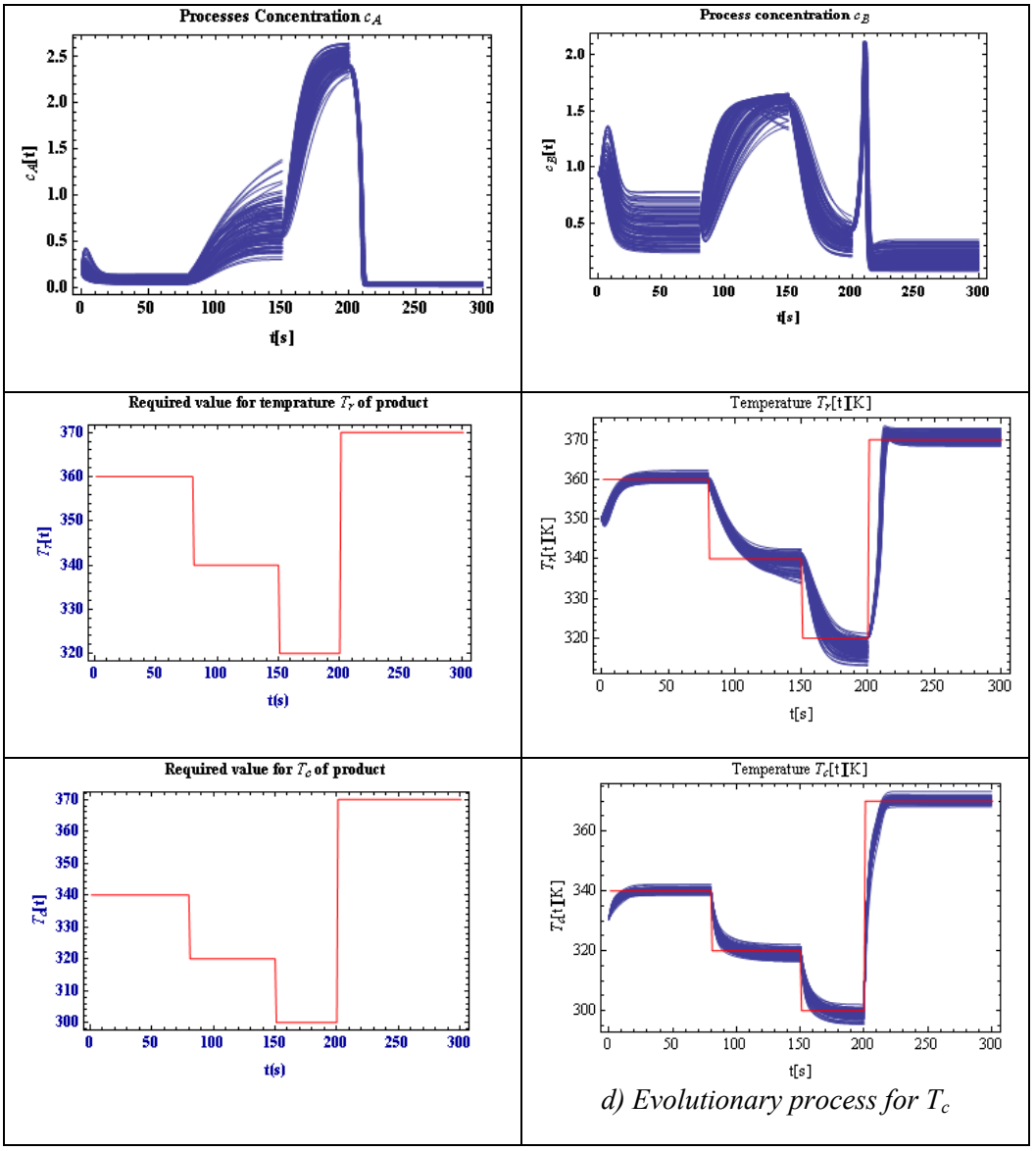


Fig. 40. Predictive control temperatures T_r and T_c of CSTR by GA, "red" was required value



d) Evolutionary process for T_c

Fig. 41. Predictive control temperatures T_r and T_c of CSTR by SA_Elitism, "red" was required value

6.4 Discussion and conclusion to the results of predictive control

The work here is performed through predictive control on non-linear system using evolutionary algorithms SOMA, DE, SA GA. Based on the achieved results it can be stated as follows:

- EA is used successfully on predictive control of the chemical reactors' processes;
- In the previous section about part optimization process of chemical reactions, it cannot be fully confirmed if any one of the chosen algorithm produced better results than the others. However, from the image results shown above, it may be concluded that SOMA and DE algorithms are best for the predictive control (at least in this case). Specifically, it can be seen in figures 38-41 items *(c)* & *(d)* for evolutionary process *Tr* and *Tc*. All 100 simulations of SOMA and DE have obtained very approximate values, which evidently prove that the courses of algorithm are densities in a thin spectrum and they meet the required value more closely than GA and SA; and
- From the results obtained, it is found that the process of concentration c_A was in inverse ratio to the process temperatures. When temperature of the reactant mixture and coolant increased, temperature of concentration c_A decreased. And when the temperature was stable, the concentration too was stable. Only on the process of concentration c_B did it appear to be failure. From interval time simulation 150-200, process of c_B decreased in direct ratio to the temperatures, and from time simulation 200, failure appeared.

Finally, it can be asserted that EAs are certainly and completely capable of controlling simple faulted system. Nevertheless, this topic deserves further and more detailed study that goes beyond the scope of the work presented here.

7 RESULTS OF DISSERTASION THESIS AND FURTHER RESEARCH PERSPECTIVE

7.1 Evaluation of the objectives

This thesis has identified six targets and the achievement of those targets are discussed here. The evaluation of each objective is contained in the information provided at the end of each chapter where the respective evaluation is carried out. Specifically:

- *The introduction of chemical engineering process, application domain of chemical reactions and reactors and analysis of chosen dynamic systems*

The objective has been achieved. In the chapter *"Chemical Engineering process"* -- it is raised that this is the important period to analyse industrial producing system, especially of chemical engineering process in the industries. This chapter confirms that the application domain of chemical reactions and reactors constitute one of the backbones for interdisciplinary collaboration. In fact, the optimization of industrial chemical processes has drawn attention in recent years, and designing the optimal parameters of reactor and its control system is one of the most difficult tasks of process engineering. Here, the thesis uses as model case, two chemical reactors, namely Batch and CSTR (known as an expert proposed), for optimization. Finding the optimum parameters of the chemical reactor and the exact procedure will greatly aid in drawing up proposal for technological equipment that can meet the economic and quality demands placed on an industrial operation.

- *Analysis of evolutionary algorithm, principle simulation and selecting new methods of algorithms, from artificial intelligence to optimization and predictive control chemical reactor.*

The objective has been achieved. Chapter 4 analysed and described very concretely about EAs and their principle in use. A brief survey of Scoping and Screening chemical reaction networks using stochastic optimization is

also raised in this chapter. Four algorithms from the field of artificial intelligence -- Differential evolution (DE), Self-organizing migrating algorithm (SOMA), Genetic algorithm (GA) and Simulated annealing (SA) -- are used in the investigation. In the first section, EAs are used investigate and optimize the batch reactor to improve its parameters. Consequently, EAs are used to model the technical requirements for chemical reaction. The second section presents the optimizing of chemical engineering processes, particularly those in which the evolutionary algorithm is used for static optimization and control of Continuously-stirred tank reactors (CSTRs).

- *Demonstrating successfully on simulation by mean evolutionary algorithms, the problem design model of chemical reactors and the practical method to optimize chemical processes.*

The objective has been achieved. In chapter 5 "Simulation part" the optimization tool has been described and four EAs were selected, especially for a certified high robustness and the ability to successfully solve complex optimization problems. Mathematical model of the process, established on the basis of balance equations, coupled with other important relationships derived for the real reactor, are used to conduct simulations of experts to set the reactor for optimization. The aim of this work was to use artificial intelligence methods, namely evolutionary algorithms, for static optimization of chemical reactor in order to improve the quality of its behaviour.

- *Demonstrating the use of designed algorithms global optimization on the predictive control chemical processes and comparing between each selected algorithms.*

The objective has been achieved. Here it is demonstrated that methods of artificial intelligence, mainly EA, are successfully applied to predictive control of a chemical reactor. The optimized reactor is used in a simulation with prediction control by evolutionary algorithms and the results are presented in graphs (see chapter 6).

7.2 General conclusion and further research perspective

In this thesis, evolutionary algorithms are used for static optimization of chemical reactors in order to improve the quality of their behaviour in the uncontrolled state and in predictive control. The optimization tool has been described and four EAs (SOMA, DE, SA and GA) are chosen, especially for a certified high robustness and the ability to successfully solve complex optimization problems of chemical reactors.

The optimization and control of the chemical reactors have been performed in several ways, each one for a different set of reactor parameters or different cost function. From the results obtained, it is possible to say that all simulations give satisfactory results and thus EAs are capable of solving this class of difficult problems. The quality of the results depends not only on the problems being solved, they are also extremely sensitive to the proper definition of the cost function and the selection of parameters setting of evolutionary algorithms.

In fact, methods of artificial intelligence, mainly evolutionary computational techniques, should be used in the difficult tasks of analysing and optimizing dynamical systems, especially of chemical reactors. The main aim of the dissertation is focused on examples of EA implementation on the methods for chemical reaction that could be robust and effective to optimize difficult problems in the field of chemical engineering, with the intent to obtain better results, i.e. efficiency in reaching the desired stable state and superior stabilization.

The basic optimization process presented here is based on a relatively simple function. Nevertheless, there is no problem in defining more complex functional including as subcriteria, e.g. stability, costs, time-optimal criteria, controllability and etc., or their arbitrary combinations; unless the experiment is limited by technical issues while searching for optimal parameters.

Future research of evolutionary algorithms SOMA, DE, GA and SA is still ongoing. Based to all results obtained from this current research, it is suggested that the main activities should be focused on the expanding of this study for other chemical dynamic systems.

It can be concluded from the results of this dissertation that EAs have shown great potential and ability to solve complex problems of optimization, not only in the fields of chemical engineering process but also in diverse industrial fields.

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[1] Tran, T.D., Zelinka, I., *Optimization of reactive distillation processes using Self-organizing Migrating Algorithm and Differential Evolution Strategies*.(14th International Conference on Soft Computing MENDEL 2008, Brno, Czech Republic, Jun 18-20, 2008. P.186-191). ISBN: 978-80-214-3675-6.

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