Applied Mathematical Modelling 37 (2013) 1137–1146

Contents lists available at SciVerse ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

A modified DNA genetic algorithm for parameter estimation of the 2-Chlorophenol oxidation in supercritical water

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ARTICLE INFO

Article history:
Received 11 July 2011
Received in revised form 16 March 2012
Accepted 21 March 2012
Available online 29 March 2012

Keywords:
DNA computing
Genetic algorithm
Parameter estimation
Supercritical water oxidation

ABSTRACT

Based on the mechanism of biological DNA genetic information and evolution, a modified DNA genetic algorithm (MDNA-GA) is proposed to estimate the kinetic parameters of the 2-Chlorophenol oxidation in supercritical water. In this approach, DNA encoding method, choose crossover operator and frame-shift mutation operator inspired by the biological DNA are developed for improving the global searching ability. Besides, an adaptive mutation probability which can be adjusted automatically according to the diversity of population is also adopted. A local search method is used to explore the search space to accelerate the convergence towards global optimum. The performance of MDNA-GA in typical benchmark functions and kinetic parameter estimation is studied and compared with RNA-GA. The experimental results demonstrate that the proposed algorithm can overcome premature convergence and yield the global optimum with high efficiency.

1. Introduction

Supercritical water oxidation (SCWO) has been widely studied and applied to the industrial organic wastewater treatment [1–3]. The design, optimization and advanced control of the SCWO process require rigorous kinetic model with precise parameters. Parameter estimation in kinetics is actually a sophisticated numerical optimization problem and has attracted considerable interests.

In the past decades, a lot of researchers have focused on using conventional optimization approaches such as the Levenberg–Marquardt (L–M), the Gauss–Newton and the Nelder–Mead algorithms to solve optimization problems [4–6]. But these deterministic optimization algorithms often get trapped into so called local optima in the search process and cannot yield satisfied results. Genetic algorithm (GA), based on the heredity and process of natural biological evolution, is one of the most important global optimization techniques. It has been successfully applied to many practical engineering problems [7–14]. Although GA has powerful global search ability and better performances compared with traditional optimization algorithms when handling complex optimization problems, it does exhibit some shortages such as premature convergence, poor exploitation capability and the convergence speed to the global optimum decreased considerably in the later period of evolution. Various attempts have been made to overcome these shortages. Many scholars find that the performances of GA critically rely on the representation of the solutions and the definition of the genetic operators. Therefore, new encoding methods and genetic operations have been employed in order to enhance the performances of GA. In [15], an improved genetic algorithm based on a novel selection strategy was presented to handle nonlinear programming problems. Valarmathi et al. [16] proposed a real-coded genetic algorithm for system identification and controller tuning in a nonlinear pH process. Inspired

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http://dx.doi.org/10.1016/j.apm.2012.03.046

by the mechanism of the biological DNA, a RNA genetic algorithm (RNA-GA) based on DNA computing was proposed by Tao and Wang for estimating the parameters of chemical engineering processes [17]. It is claimed that the accuracy and the diversity of the population have been improved significantly by encoding chromosomes with nucleotide bases and adopting some RNA molecular operations. Wang and Wang also proposed a novel RNA genetic algorithm (NRNA-GA) and a protein inspired RNA genetic algorithm to estimate the parameters of dynamic systems [18,19]. Chen and Wang developed a DNA based genetic algorithm, which adopts new genetic operators, to determine 25 kinetic parameters of hydrogenation reaction successfully [20].

In order to improve the search efficiency and prevent premature convergence, we present a modified DNA genetic algorithm (MDNA-GA). Further, this method is applied to five benchmark test functions and the kinetic parameter estimation of the 2-Chlorophenol oxidation in supercritical water.

2. Implementation details of MDNA-GA

2.1. Representing and decoding

The global optimization problem can be expressed as follows:

$$\begin{aligned} &\min f(x_1, x_2, \ldots, x_n), \\ &\text{s.t.} \quad x_{jmin} \leqslant x_j \leqslant x_{jmax} \quad j \in \{1, 2, \ldots, n\}, \end{aligned} \tag{1}$$

where $f(\boldsymbol{x})$ denotes the objective function, $\boldsymbol{x} = \{x_1, x_2, \ldots, x_n\}$, x_j is a variable to be optimized, x_{jmin} and x_{jmax} represent the inferior and the superior bounds of x_j respectively.

When applying MDNA-GA to a global optimization problem, it is necessary to determine the representing scheme for chromosomes. DNA, the hereditary material that contains plentiful genetic information necessary for almost all living organism, is composed of units called nucleotides. There are four different types of nucleotides found in DNA, differing only in the nitrogenous base, two are purines, adenine (A) and guanine (G), and two are pyrimidines, cytosine (C) and thymine (T). Inspired by DNA molecular structure, we use nucleotide bases A, G, C, and T, to encode the possible solutions of the optimization problem. To perform calculations conveniently, four bases should be represented by numbers. Therefore, integer 0, 1, 2, and 3 are adopted to encode four nucleotide bases. The mapping from nucleotide bases to the integer is represented as C-0, T-1, A-2, G-3.

Based on the encoding scheme described above, every variable x_j of the given problem is represented as an integer substring of a specified length l. Thus a chromosome of the n-variable optimization problem is encoded into an integer string with the length $L = n \times l$.

The procedure of decoding can be described as follows:

First, each chromosome is separated into n parts, for part j, the substring of variable x_j will be converted to an integer value according to the following formula:

$$intx_j = \sum_{p=1}^{l} bit(p) \times 4^{l-p}, \tag{2}$$

where $bit(p)$ is the digital number of the pth gene for x_j, $int\ x_j$ is a decimal integer, and $0 \leqslant int\ x_j \leqslant 4^l - 1$. The range of variable x_j is $[x_{jmin}, x_{jmax}]$, and then each interval is divided into $4^l - 1$ sub-intervals. The length of sub-interval of x_j can be calculated as $\Delta_j = (x_{jmax} - x_{jmin})/(4^l - 1)$. Hence, $intx_j$ will be mapped into a real number x_j:

$$x_j = x_{jmin} + \Delta_j \times intx_j. \tag{3}$$

2.2. Design of genetic operators

We adopt the genetic operators including reproduction, crossover and mutation are described as follows.

2.2.1. Reproduction

Reproduction is the process which stochastically selects the individuals from the population according to their fitness values. There are three main types of selection methods: roulette wheel selection method, ranking method and tournament selection method. Tournament selection is adopted as the individual selection instrument for the reproduction process in this paper. Two individuals are randomly chosen among the population and compared their fitness values. Then the individual with greater fitness value is allowed to be copied into the next generation. Elitism strategy is employed to prevent the loss of the best individual during evolution.

2.2.2. Choose crossover operator

The crossover operation is mainly responsible for the global searching ability of the algorithm. Once the new population is formed by selection operation among the previous population, the crossover operation is implemented by exchanging information between two randomly selected parent individuals from the current population.