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A protein inspired RNA genetic algorithm for parameter estimation in hydrocracking of heavy oil

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ABSTRACT

Hydrocracking is a crucial process in refineries and suitable model is useful to understand and design hydrocracking processes. Simulating the procedure from RNA to protein, a protein inspired RNA genetic algorithm (PIRGA) is proposed to estimate the parameters of hydrocracking of heavy oil. In the PIRGA, each individual is represented by a RNA strand and a new fitness function combining traditional fitness value and individual ranking is employed to maintain population diversity. Furthermore conventional crossover operators are replaced by RNA-recoding operator and protein-folding operators to improve the searching ability. An adaptive mutation probability in the PIRGA makes the algorithm have more chance to jump out of local optima. Numerical experiments on seven benchmark functions indicate that the PIRGA outperforms other genetic algorithms on both convergence speed and accuracy greatly. 10 parameters are obtained by the PIRGA and the kinetic model for hydrocracking of heavy oil is established. Experimental results reveal that the predictive values are in good agreement with the experimental data with relative error less than 5%. The effectiveness and the robustness of the model are also validated by experiments.

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1. Introduction

The conflict of growing demands of middle distillates with overabundance of heavy crude oils makes people focus on hydrocracking technique and hydrocracking is increasingly becoming a crucial secondary petroleum refinery processes to treat heavy oil, such as vacuum resid. The main objective of this process is to convert heavy molecules like vacuum gas oil (VGO) into lighter and more valuable fractions such as naphtha, gasoline, and hydrogen gas. Different approaches have been utilized for kinetic modeling of hydrocracking, varying from the most common and used lumping technique to more complex models based on continuous mixture or single events. A comprehensive review of hydrocracking modeling can be found in [1].

Accurate analytical or numerical modeling of these new upgrading processes is essential, in order to correctly interpret experiment measurements and to lead to a better understanding and design of industrial-scale processes. However, many undesirable and complicated reactions in hydrocracking process bring an arduous task to make a reasonable tradeoff between accuracy and complexity of modeling. Usually, people consider these reactions dominant and significant in all reaction and neglect tiny ones. After getting mechanism model of hydrocracking processes, determination of model parameters is also difficult by conventional deterministic optimization methods [2]. Most deterministic optimization methods encounter some deficiencies such as sensitive to initial value and/or requiring of differentiable information of optimized problems.

Genetic algorithms (GAs) first developed by Holland are stochastic search technique based on the mechanism of natural selection and survival of the fittest [3,4]. Those individuals with higher fitness value are assigned higher survival probability. Genetic algorithms do not tackle problems directly but in a chromosome space, i.e., candidate solutions of an optimization problem are converted to chromosome firstly. Due to no requirement of prior information about search space and owning excellent global search ability, GAs have been applied widely to address complicated real-world problems with non-differentiable, non-convex and non-linear [5–10].

Despite successful applications of GAs to optimization problems, traditional genetic algorithms suffer from slow convergence speed and poor local searching ability. Furthermore, simple operators of GAs limit their searching efficiency in searching space and redundant search dominates the whole procedure. In order to overcome these drawbacks of GAs, some improved genetic algorithms simulating biological behavior emerged. Inspired by DNA molecular structure and operators, Tao et al. proposed a RNA genetic algorithm, which adopts quaternary encoding and three RNA molecular operators to improve the searching capability of GAs [11]. Wang et al. presented a novel RNA genetic algorithm to

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Nomenclature

N	population size
M	individuals number in mating pool
l	length of RNA individuals
F_i	original fitness value of individual i
F_i'	new fitness value of individual i
R_i	ranking number of individual i
N_{best}	population size of neutral group
n_1	number of left-shift steps
n_2	number of right-shift steps
$P_{\text{RNA-recoding}}$	probability of RNA-recoding operator
$P_{\text{mutual-folding}}$	probability of protein mutual-folding operator
$P_{\text{self-folding}}$	probability of protein self-folding operator
P_m	mutation operator probability
$G_{\max}$	number of maximal generations
D	dimensions of benchmark functions
g	generation number
VGO	vacuum gas oil
r_i	reaction rate of product composition i
ω_i	mass fraction of product composition i
E	relative error
T_0	starting time of collecting data
T_t	stopping time collecting data
$y_i(nt)$	experimental data of composition i at time of nt
$\hat{y}_i(nt)$	predictive value of composition i at time of nt

make a reasonable tradeoff between searching accuracy and computational efforts by introducing a new RNA molecular operator, stem-loop operator, and two different fitness values. Computational results showed that this RNA genetic algorithm solved three parameter estimation problems of dynamic systems successfully [12]. Chen et al. developed another DNA genetic algorithm to address parameter estimation problem in hydrogenation reaction well [13]. Tao et al. and Chen et al. suggested two different hybrid genetic algorithms incorporating DAN double helix genetic algorithm and sequential quadratic programming (SQP) for gasoline blending scheduling problems [14,15].

Simulating RNA molecular operators and procedure from DNA to protein in biological cell, a protein inspired RNA genetic algorithm (PIRGA) is proposed in this work. In this algorithm, we first encode each individual with a strand of nucleotide bases, RNA strand. Then RNA-recoding operator and protein-folding operators are designed to replace conventional crossover operators to improve the performances of GAs. Apart from encoding procedure, RNA strands are first translated into amino acids ones, protein strands, according to triplet codons in decoding procedure. Numerical solutions on seven benchmark functions, varying from two-dimensional to ten-dimensional, show the superiority of the PIRGA in contrast to other genetic algorithms. The parameters estimation problem in hydrocracking kinetic model is also well addressed by the proposed genetic algorithm.

2. Protein inspired RNA genetic algorithm (PIRGA)

2.1. Representing and decoding

DNA is the major genetic material for life and contains plentiful genetic information. DNA molecular owns a double helix structure and during DNA replication and transcription, the double helix must be separated transiently and reversibly. Because the separated antisense strand, RNA individual, contains almost all useful information of DNA and is simpler on structure than DNA molecular, RNA is also regarded as main genetic material of living cells. RNA contains 4 kinds of nucleotides: Adenine (A), Uracil (U), Guanine (G) and Cytosine (C). In the PIRGA, all individuals are represented by RNA strands and the encoding space is $E = \{A, U, G, C\}^l$, where l is the length of RNA strands (All strands are the same length in the PIRGA).

Table 1
Relationship between triplet codons and 64-ary integers.

First nucleotide	Second nucleotide				Third nucleotide
	U	C	A	G	
U	0	4	8	12	U
U	1	5	9	13	C
U	2	6	10	14	A
U	3	7	11	15	G
C	16	20	24	28	U
C	17	21	25	29	C
C	18	22	26	30	A
C	19	23	27	31	G
A	32	36	40	44	U
A	33	37	41	45	C
A	34	38	42	46	A
A	35	39	43	47	G
G	48	52	56	60	U
G	49	53	57	61	C
G	50	54	58	62	A
G	51	55	59	63	G

In genetic code, a three-letter codes, triplet codon, decides a amino acid, i.e., three nucleotides in RNA strand decide a amino acid by the translating operator. On the decoding procedure of the PIRGA, RNA strands are first translated into amino acid strands, protein ones. In biological field, 20 kinds of common amino acids are recognized by codons, and some different triplet codons decide the same amino acid. Though the degeneracy of triplet encoding in cell plays an important role in reducing replication error and abnormal mutation, in GAs we hope individuals and candidate solutions are one–one relationship which can reduce computational costs in searching procedure. Hence on decoding procedure, RNA strands are first translated into 64-ary. The relationship between triplet codons and 64-ary integers is shown in Table 1.

After translating operator individuals are represented by amino acid ones, i.e., integer sequences between [0,63] which are easy to convert to real-values in domain of an optimization problem. This indirect decoding method first translates RNA individuals into amino acid sequences and then these 64-ary amino acid strands are converted to real-values. The length of RNA individuals is decided by variable number of problem and precision. For example, there are n variables and each variable is represented by m 64-ary integer. The length of RNA individuals is $l = 3 \times n \times m$. The decoding procedure is shown in Fig. 1.

Encoding procedure is a mapping from solution space to RNA encoding space, i.e., RNA strands are adopted to represent individuals in the PIRGA. Subsequently, these RNA individuals change their forms in the encoding space by some RNA and protein molecular operators. When the algorithm terminated, Optimization results are obtained by decoding procedure, which is an inverse mapping from RNA space to problem space. In other words, the encoding and the decoding procedures complete a mutual mapping between solution space and RNA operator space.

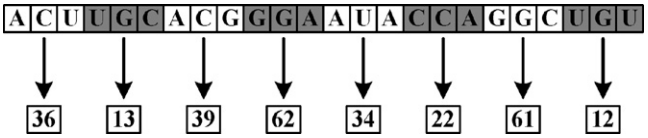

Fig. 1. Decoding procedure.

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