THE USE OF OPTIMIZATION IN FIRE DEVELOPMENT MODELING
The Use of Optimization Techniques for Estimation of Pyrolysis Model Input Parameters

Jiří Ira[a], Lucie Hasalová[a], Milan Jahoda[a]

[a] Institute of Chemical Technology, Praque, Faculty of Chemical Engineering, Praque, Czech Republic

Abstract
This paper deals with the use of the optimization techniques for obtaining the input parameters from the bench scale experimental data that are used for property based fire modeling. Two multidimensional optimization techniques - Genetic algorithm (GA) and Shuffled complex evolution (SCE) - are discussed. Their performance is compared based on the algorithms application to estimation of the material properties of one of the commonly used structural materials – wood.

Keywords: fire modeling, genetic algorithm, material properties estimation, global optimization, shuffled complex evolution, wood

INTRODUCTION

CFD fire modeling quickly emerged as an useful and nowadays quite common tool in fire and safety engineering practice. Commercially affordable CFD fire modeling softwares as FDS, Jasmine or SmartFire are successfully used in many key fire safety applications, e. g. proposing fire evacuation strategies, designing the layout of the active fire protection components etc., where the main objective of the model is to study the consequences of the fire (mainly the evolution of the temperature field and spread of the smoke). When the amount of the heat released during burning (HRR) is known, commercial fire modeling softwares provide good agreement between the model and the real case situations and work as a reliable prediction tool.

Contrary to fire consequence modelling, capabilities of the softwares in case of fire development and spread modelling are still very limited and their use is restricted to research area only. The main challenge in modeling fire spread is to accurately predict the amount of the mass released when the material is exposed to heat as a function of time, i.e. to establish the pyrolysis model together with an appropriate reaction scheme of the material heat degradation.

Considering the basic construction materials, the knowledge of the material mass loss rate when exposed to heat is crucial from the point of view of the buildings static. The amount and the composition of the gases released during pyrolysis significantly influence the evolution of the temperature field and the rate of the heat transfer to the surrounding materials. High temperatures further initiate pyrolysis and leads to the irreversible damage of the building structures (the loss of strength and stiffness of steel beams or the destruction of the concrete components caused by the sudden release of the water vapour from the moisture present in the concrete).

When modeling pyrolysis the main problem is not the insufficient theoretical knowledge of the pyrolysis models, but the lack of the methodology how to determine the model input parameters – kinetic and thermal parameters of the decomposing material. Some of the material properties can be determined from the experimental measurements like thermogravimetric analysis (ISO, 1997), conic calorimetry (ISO, 2002) or differential scanning calorimetry (ISO, 2009). However, most of the parameters have to be determined by

inferring or optimization from the experimental data. The paper deals with using optimization techniques for estimating the pyrolysis model input parameters.

1 THE PYROLYSIS MODELING

FDS (McGrattan et al., 2010), Gpyro (Lautenberger, 2007) and Thermokin (Stoliarov & Lyon, 2008) belong currently to the most common pyrolysis models in the fire community. Although these models were developed independently, their mathematical formulation are quite similar. The main differences between the models are the variable specification (e.g. conversion) and the extent of their generality. One of the key governing equations in the pyrolysis model are the condensed phase mass conservation and the condensed phase species conservation. These equations describe the change of the mass of the condensed phase over time in the computational cell, i.e. how quickly the condensed phase species are released into the gas phase. One of the ways to express a mass change is the use of conversion. Therefore the reaction rate of species decomposition is the function of thermodynamic temperature *T* and conversion α (normalized mass fraction). For simplifying the reaction rate is usually expressed as the product of two independent functions

$$r = k(T)f(\alpha) \tag{1}$$

where $f(\alpha)$ is only a function of conversion and $k(T)$ is only a function of temperature. The dependence of the reaction rate on temperature is usually expressed by the Arrhenius equation. The function $f(\alpha)$ is called "reaction model" and may have different forms. The simple form $(1-\alpha)^n$ is most commonly used. Than the equation for description of the condensed phase decomposition kinetics has this basic form

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = Z\exp\left(-\frac{E}{RT}\right)(1-\alpha)^n \tag{2}$$

where *Z* is the pre-exponential (frequency) factor, *E* is the activation energy, *R* is universal gas constant and *n* is the reaction order. The Arrhenius equation parameters (Z, *E*) together with the reaction order *n* are input parameters into models of thermal decomposition of solid materials.

1.1 The optimization techniques

The problem of determination of material pyrolysis properties from bench-scale experimental data is an inverse problem. The major complications for solving the inverse problem are the existences of more than one main convergence region and many minor local optima in each region. In general there are many approaches how to solve such global optimization problem (e.g. deterministic methods, stochastic methods, heuristics etc.), but not all can be applied to this problem. The main concern when choosing the optimization method is how close the converged solution is to the global optimum and how quickly the algorithm converge to a solution.

Since 1998, several scientific workers tried to apply different optimization algorithms to the inverse problem of pyrolysis parameters estimation. One of optimization algorithms tested through the fire research community was the genetic algorithm (GA) that belongs to the group evolutionary algorithms. Genetic algorithm is heuristic method that uses the principles of evolutionary biology (natural selection, crossover, mutation, heredity) to find the global optimum. The basic principle of genetic algorithm is described in Fig. 1a. Although the GA was proofed to be very versatile and powerful tool its use has a number of disadvantages. Results obtained by GA are strongly dependent on the initial setup of algorithm parameters such as population size, mutation probability, crossover probability or selection mechanism. Moreover, the GA may have a problem with finding the global optimum. If we change one (or more) parameter we can get qualitatively different solution which meet the optimization criteria as well.

Chaos et al. (2010) used the shuffled complex evolution (SCE) algorithm to estimate the material pyrolysis properties from FPA (ISO, 2011) experimental data. The shuffled complex evolution is the global optimization algorithm developed by Duan et al. (1993) at The University of Arizona. The SCE method combine the strength of Nelder-Mead (downhill simplex) method, controlled random search, genetic algorithm and complex shuffling. The flowchart of SCE algorithm is shown in Fig. 1b. Lautenberger (2011) implemented the SCE algorithm to his pyrolysis model Gpyro and compared its performance over GA using synthetic cone calorimeter experimental data of hypothetical non-charring material. The result suggested that in comparison to GA, SCE converge to a unique solution that corresponds to the global optimum. The normalized deviation between solution was not usually greater than units percent. Moreover, the fitness function reached much higher values (the fitness function is maximized). However, to confirm these conclusions SCE need to be further tested. It is necessary to apply the SCE on various materials and decomposition patterns.

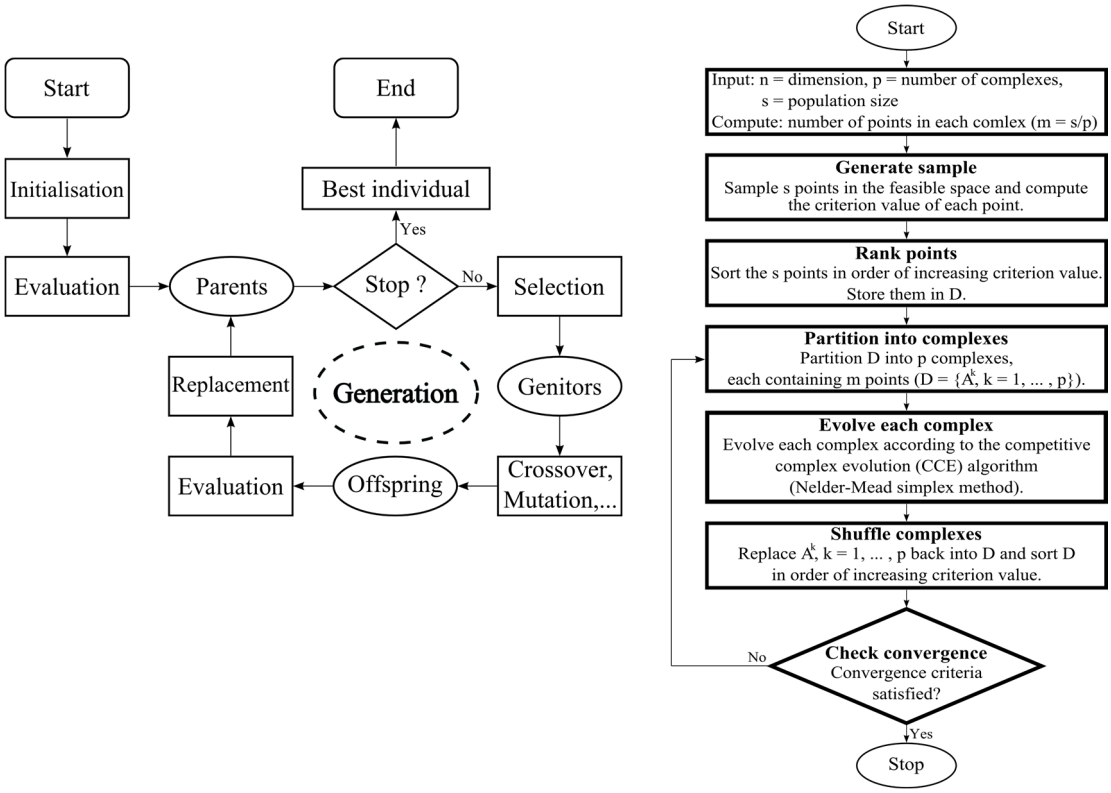

Fig. 1 Optimization algorithm flowcharts a) GA, b) SCE

2 COMPUTATIONAL PART

This work deals with the estimation of beech wood decomposition kinetics using GA and SCE optimization algorithm. The experimental data used for the optimization routine were obtained from thermogravimetric analysis (TGA). TGA was carried out in nitrogen atmosphere with heating rate of a sample 5 K/min to the maximum temperature 800 °C.

For the thermal decomposition of beech wood in non-oxidative atmosphere three-step reaction scheme was chosen, shown in Fig. 2. In the first step the water vapour naturally contained in the wood evaporates resulting in the change of the wood density. Subsequently the dry wood decomposes by two independent reactions forming char and gaseous pyrolysate. In the last step, the char transforms to residue again releasing gaseous pyrolysate.

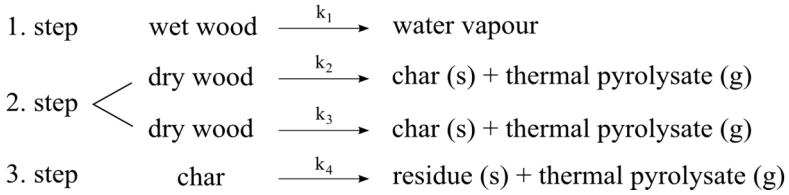

Fig. 2 Beech wood thermal decomposition reaction scheme

For the selected model the total number of parameters to be estimated is 14. 12 parameters (*Z*, *E*, *n* for each decomposition reaction) are kinetic parameters for reaction k_1, ..., k_4 and the remaining two are the density of char and the density of residue.
The estimation of the set of 14 parameters was carried out in program Gpyro. To determine the model kinetic parameters two global optimization methods - genetic algorithm and shuffled complex evolution - were chosen.
One of the main goals of the this work was to assess the ability of the optimization algorithm to converge to the unique solution. Therefore ten trials with different initial parameter values randomly generated in the search parameter space (specified by user) were performed both using GA and SCE. At the end model data computed using both GA and SCE estimated parameters were compared to the experimental TGA results. Additionally the rate of convergence and final average value of fitness function were studied to compare which of the algorithms is computationally more efficient.
To investigate the influence of the population size using GA, four calculations with the population size doubling in every run from 125 to 1000 individuals were performed.

3 RESULTS

The sets of parameters obtained by optimization using both GA and SCE are summarized in Tab. 1. The parameters listed here are the boundaries of each variable search space, the average values of individual variables calculated from 10 trials with different initial estimate of the parameter values, absolute standard deviation from the average value and normalized standard deviation from the average value in percentages.

Tab. 1 GA settings: 250 individuals, 200 generations, SCE settings - 8 complexes each with 29 points, i.e. 232 points in total

			Boundaries		**GA**			**SCE**		
Number	**Variable**	**Units**	**Minimum value**	**Maximum value**	**Average**	**Absolute standard deviation**	**Norm. st. dev. (%)**	**Average**	**Absolute standard deviation**	**Norm. st. dev. (%)**
1	$\log Z_1$	$\log s^{-1}$	3.5	5.0	4.03	0.39	9.64	3.87	0.22	5.81
2	E_1	kJ/mol	35.0	50.0	45.9	2.1	4.57	44.1	2.2	4.98
3	n_1	-	0.7	1.5	1.14	0.16	14.21	1.39	0.13	9.27
4	$\log Z_2$	$\log s^{-1}$	10.5	12.5	11.40	0.31	2.72	11.81	0.48	4.05
5	E_2	kJ/mol	140.0	160.0	151.0	3.3	2.17	155.5	4.9	3.17
6	n_2	-	1.4	3.0	2.18	0.14	6.35	2.13	0.11	5.33
7	$\log Z_3$	$\log s^{-1}$	19.0	21.0	19.84	0.27	1.34	19.14	0.27	1.41
8	E_3	kJ/mol	250.0	280.0	262.5	2.8	1.08	255.0	3.1	1.22
9	n_3	-	1.0	2.0	1.79	0.17	9.37	1.66	0.10	5.80
10	$\log Z_4$	$\log s^{-1}$	6.0	9.0	6.99	0.38	5.46	6.64	0.14	2.07
11	E_4	kJ/mol	140.0	170.0	149.9	4.3	2.86	141.0	2.2	1.54
12	n_4	-	2.0	3.5	3.10	0.32	10.19	3.50	0.00	0.11
13	ρ_{char}	kg/m^3	80.0	200.0	196.3	3.1	1.58	198.5	1.53	0.77
14	$\rho_{residue}$	kg/m^3	80.0	200.0	166.4	1.5	0.90	165.7	0.57	0.34
					Absolute average:		**5.17**			**3.28**

It can be seen, that both algorithms converged to one same solution within deviation of approximately 5.2 and 3.3 % using GA and SCE respectively. The highest normalized standard deviation from all parameters was approximately 14.5 % with GA and 9.5 % with the SCE algorithm both in the same parameter - reaction order of the first reaction.
In overall, SCE performed slightly better than GA, but our calculations did not confirm that GA should have a problem to find qualitatively the same solution. The Fig. 4 and Tab. 1 suggest that the GA is also able to find "one" solution for our case. This may be due to the fact that the parameter space is very closely specify and does not have to contain a large number of local extremes. However, definition of the close parameter space requires extensive user experience.
The disadvantage of using the real experimental data is, that the exact values of the material parameters are not known, so it is not possible to assess the accuracy of the results. However it is possible to compare the model results using average values from Tab. 1 with the experimental data to verify whether the estimated parameters provide a good fit (Fig. 3). As can be seen, the selected reaction model can describe the experimental curves very well. It describes both the initial mass loss and the secondary peak in the MLR curve.
Fig. 4a shows the GA fitness evolution of the ten trial computations. The group of curves with higher fitness represent the evolution of the best individual (the individual with the highest value of fitness function from all individuals) in the population. The curves below describe average fitness value in the population. For the relatively small population (250 individuals and less) oscillations of fitness function occurs. The part of GA as the evolutionary algorithm are the random processes (e.g. mutation) which can cause that the best individual is knocked out of the population and the fitness function with the number of function evaluations actually decreases.
The SCE fitness evolution for ten different trials with the different random number seeds is shown in the Fig. 4b. Opposed to GA, the SCE fitness evolution is much smoother and without oscillation. The fitness function value increases rapidly in the first approximately 5000 function evaluations and then slowly increase. The fitness evolution follows quite similar pattern in all trials and the fitness level reaches the absolute higher value than in GA.
Fig. 5 shows the effect of population size in the GA on the fitness evolution. With the increasing population size the rate of convergence decrease and decrease the frequency of oscillation - the probability that the best individual will be randomly eliminated decreases with increasing population.

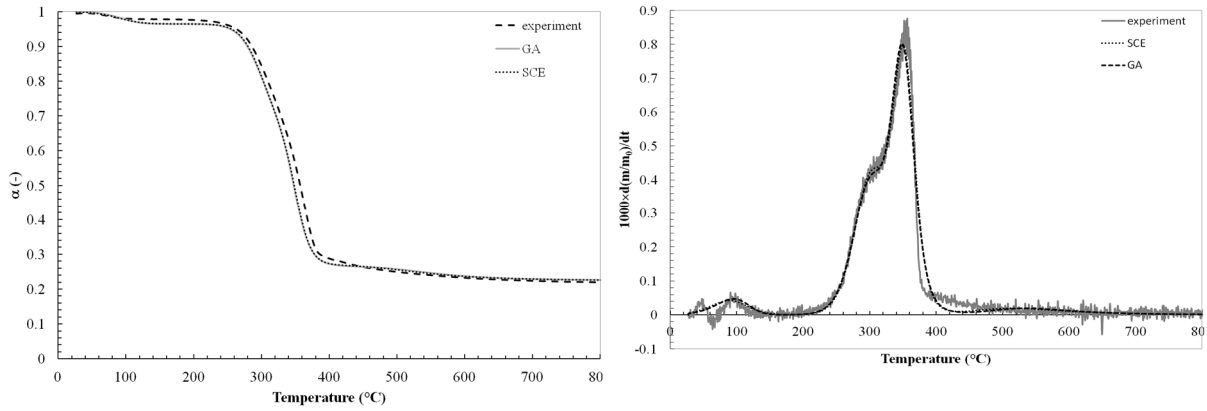

Fig. 3 Comparison of the experimental and model data

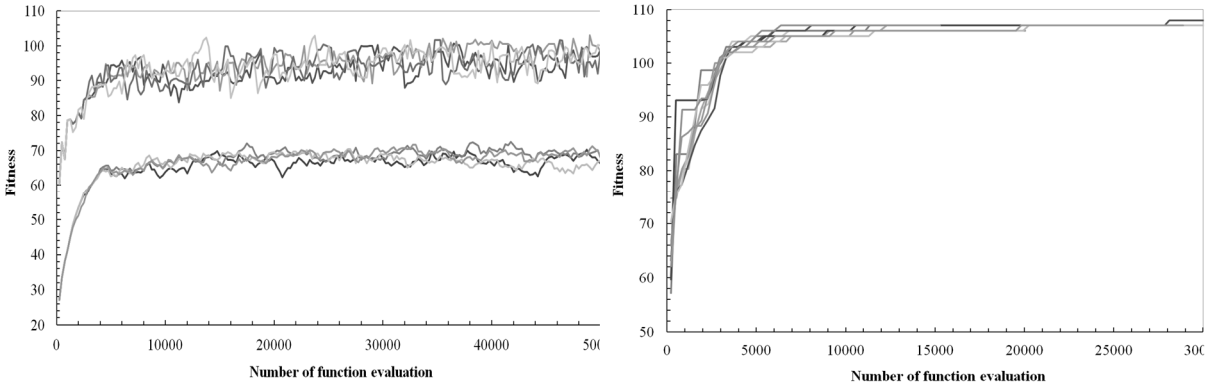

Fig. 4 Fitness evolution a) GA, b) SCE

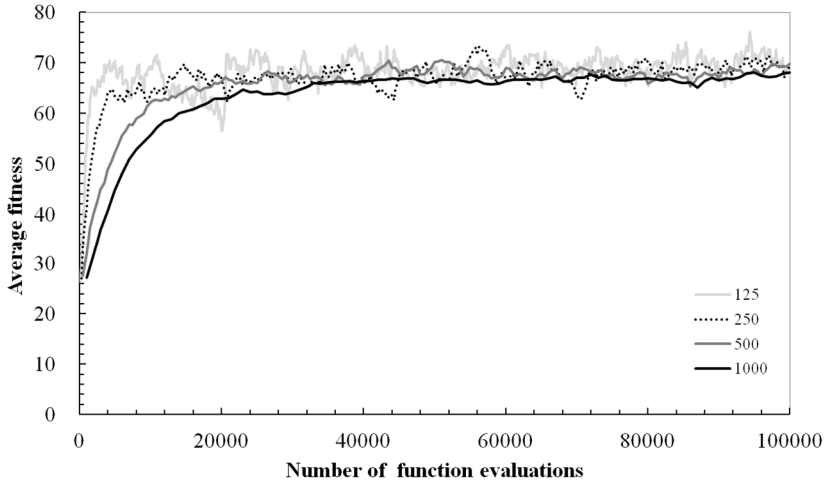

Fig. 5 GA fitness evolution for various population size 125, 250, 500 and 1000 individuals

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