Conjugate Direction Particle Swarm Optimization Based Approach to Determine Kinetic Parameters from Part of Adiabatic Data

Xiao-Qiao Zhao, Hao Wang, Wen-Qian Wu, and Wang-Hua Chen

Abstract—Due to the limited detection range of the adiabatic equipment, it is difficult to get complete experimental curve of some materials and calculate the kinetic parameters. In this work, the conjugate direction particle swarm optimization (CDPSO) approach, as a global stochastic optimization algorithm, is proposed to estimate the kinetic parameters and complete experimental curve from part of adiabatic calorimetric data. This algorithm combines the conjugate direction algorithm (CD) which has the ability to escape from the local extremum and the global optimization ability of the particle swarm optimization (PSO) which finds the globally optimal solutions. One case was used to verify this method: 20% DTBP in toluene decompositions under adiabatic conditions. Comparing the experimental and calculated complete temperature curve, the accuracy of the fitted kinetic parameters calculated by no less than 70% temperature rise rate proportion of data is verified. The value of TD24 is well-deviated even used 10% proportion of data. The case reasonably proves the effectiveness of CDPSO algorithm in the estimation of kinetic parameters from part of adiabatic data.

Index Terms—Conjugate direction particle swarm optimization, Kinetic parameters, part of adiabatic data, 20% DTBP, T_{D24} .

I. INTRODUCTION

Adiabatic calorimetry is well known as one of the main methods for kinetics evaluation. The kinetics evaluation is very useful for simulation-based assessment of reaction hazards [1], simulation of undesired behavior for a large reactor or the whole process [2], optimization of the chemical process [3], safety analysis of storage and transportation of a chemical product, and so forth.

The reliability of kinetics evaluation obtained is determined by valid kinetic model and accurate experimental data. Different kinetic models should be considered to analyze different kinds of reaction [4], [5]. The most extensively used is N-order reaction model. Due to the intense non-linear characteristics of the kinetic model under adiabatic conditions, estimation of the kinetic parameters is usually based on nonlinear optimization algorithms. For common gradient-based optimization algorithms, like Newton–Gauss method, Tensor method, it is difficult to find the true direction to the global minimum when the initial guess is located far from the global minimum. Therefore, Guo Zichao *et al.* [6] reported a method to evaluate globally optimal kinetics by a hybrid Particle Swarm Optimization (PSO) algorithm which is more efficient. However, it requires fewer number of function evaluation, while leading to better or the same quality results. Due to the limited range of the adiabatic equipment or mistake of experimental conditions setting, it is difficult to get complete experimental curve of some materials. Although PSO is well suited to evaluate kinetics with accurate experimental data, the ability to calculate kinetics with incomplete data is weak.

It is accepted that the Conjugate direction (CD) method, a nonderivative optimization method proposed by Powell [7], has a strong ability to optimize local solution for multi-dimensional situation. Therefore, in this work, the conjugated direction particle swarm algorithm (CDPSO) will be employed to estimate the kinetic parameters with incomplete adiabatic data. The proportion of incomplete data in the whole adiabatic data is required.

Studies of two case will be conducted to validate the CDPSO method and find the critical proportion of adiabatic data from two aspects of temperature rise and time point.

II. THE CONJUGATED DIRECTION PARTICLE SWARM OPTIMIZATION (CDPSO)

A. Particle Swarm Optimization

Particle Swarm Optimization (PSO) was proposed by Kennedy and Eberhart [8]-[10] and it is a bionic algorithm that mimics the foraging behavior of birds. The basic formulas are as follows:

$$v_{t+1}^{i} = \omega v_{t}^{i} + c_{1} \varphi_{1} \left(p_{\text{best}}^{i} - x_{t}^{i} \right) + c_{2} \varphi_{2} \left(p_{\text{best}}^{g} - x_{t}^{i} \right)$$
(1)

$$\mathbf{x}_{t+1}^{i} = \mathbf{x}_{t}^{i} + \mathbf{v}_{t+1}^{i} \tag{2}$$

where *t* denotes the number of iteration, x_t^i denotes the position of particle i at iteration *t*, v_t^i denotes the velocity of particle *i* at iteration *t*, x_{t+1}^i is the position of particle *i* at iteration t+1, v_{t+1}^i denotes the velocity of particle *i* at iteration t+1, w_{t+1}^i denotes the velocity of particle *i* at iteration t+1, ω , c_1 and c_2 are three adjustable parameters. φ_1 and φ_2 are random number of (0, 1). p_{best}^i is the best position of particle *i* in the past iterations, p_{best}^g is the best position in the past iterations in the group. The position and velocity update process of particles are depicted in Fig. 1.

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Fig. 1. The position and velocity update of particles.

However, PSO is easy to be trapped into local minima in optimizing high-dimensional function. Lots of improved method had been proposed, including improving the control parameters or combining with another algorithm.

B. Conjugate Direction Algorithm

Conjugate direction (CD) method was proposed in 1964 by Powell [7]. It can get a better optimization solution than using PSO alone. CD algorithm is an optimization algorithm and it does not require derivation of the objective function with the basic steps of this algorithm as followed:

Step 1. A random point A is taken as the initial point, and the n coordinate axes are taken as the initial linearly independent directions. Each optimization solution is taken as the initial position for the next optimization arbitrarily from point A and produce the optimal point B. Then point B denotes the final solution and the iteration number k is equal to 0.

Step 2. The point *B* is taken as the initial position and optimize the objective function along n coordinate axes by linearly search method. When all of the n directions have been searched, we get the last point *C*. It has been proved that the new direction of BC must be conjugate with the first coordinate axis. Then BC is taken to be the new direction and get an optimal point E from point *C* and n directions. the iteration number *k* is equal to k+1.

Step 3. The point E is set as the initial position. Then go to step1 and repeat the loop with iteration number k equal to k+1. Finally, it gets the optimization solution D until k=n. The point D must be closer to the optimal solution than point A.

C. Conjugate Direction Particle Swarm Optimization

PSO is a random algorithm with arbitrary initial particles. Because the initial particle is more than one particle, the optimization value of the objective function will decline rapidly at the beginning. After several iterations, the decline velocity would reduce, and eventually may fall into a local minimum, especially if it is a high-dimensional optimization case. Therefore, conjugate direction method is applied with conjugate direction method that can get a better certain initial point and quickly converge. However, it may take a long time to calculate to get an appropriate initial point and it would even fail sometimes [11].

Conjugate direction particle swarm optimization (CDPSO) has advantages of the above two algorithm. At the configuration stage, after 50 random initial particles

generated, the corresponding values of objective function are calculated. The best particle in the group is taken as P_{Best} . Then it goes into the PSO stage. When the particle falls into a local extremum, PSO stage stops. Next it goes into the CD stage with the initial particle $P_{\text{Best},\text{PSO}}$. a better solution ($P_{\text{Best},\text{CD}}$) is found out of the local extremum value. If the fitting correlation coefficient of the optimization value is higher than 0.9999 or the optimization loop again is until 4 iterations, P_{Best} , will be output. The process of CDPSO is illustrated in Fig. 2.



Fig. 2. The flowchart of CDPSO used in this work.

III. KINETICS

For the specific ARC test, all heat generated by the reaction is used to heat up sample container and sample. In accordance with the first law of energy conservation, the conversion rate at any reaction time, α_t , can be calculated by

$$\alpha_t = \frac{Q_t}{Q^{\infty}} = \frac{T_t - T_{\rm on}}{T_{\rm f} - T_{\rm on}} \tag{3}$$

The reaction rate can be quantitatively expressed using the Arrhenius linearization method.

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = k_0 e^{-E/RT} f(\alpha) \tag{4}$$

where k_0 is the pre-exponential factor, E is the activation energy and $f(\alpha)$ is mechanism model, R is the ideal gas constant. For a single-stage of N-order reaction, $f(\alpha)$ is shown as Eq. (5).

$$f(\alpha) = (1 - \alpha)^n \tag{5}$$

For an adiabatic reaction system, the temperature rise rate can be deduced from the conversion rate and the Arrhenius linearization method.

$$\frac{\mathrm{d}T}{\mathrm{d}t} = k_0 e^{-E/RT} \Delta T_{ad} \left(1 - \alpha\right)^n \tag{6}$$

In this kinetic model, the model parameters k_0 , E, n and ΔT_{ad} will be selected as the variables and simultaneously estimated by the CDPSO algorithm.

IV. EXPERIMENT

A. Sample

Solution of 20% di-tert butyl peroxide in toluene (20% DTBP) [12], [13], was purchased from Aldrich. Dicumyl peroxide, DCP (99% purity) in the form of white crystalline solid substances was procured from Shanghai Ling Feng Chemical Reagent Co. Ltd. China. The two samples were stored in a refrigerator at 4°C and used without more purification.

B. ARC Test

esARC was manufactured by Thermal Hazard Technology Company in Britain and the measurement temperature range is from 30 to $450 \,\text{C}$, pressure can be logged from 1 to 150 bar and the sensitivity of temperature measurements is $0.02 \,\text{C} \,\text{min}^{-1}$.

The test conditions and measured parameters are summarized in Table I.

TABLE I: ARC TEST RESULTS FOR DTBP-TOLUENE MIXTURE

m _{sample}	m _{bomb}	$C_{p,sample}$	$C_{p,bomb}$	φ	T_{onset}	$T_{ m final}$
(g)	(g)	(J/(g•K))	(J/(g•K))		(°C)	(°C)
4.95	13.32	2	0.42	1.56	115.36	181.77

TABLE II: COMPARISON OF THE KINETIC PARAMETERS BETWEEN THIS WORK AND OTHER WORKS FOR 20%DTBP

	K_0 , s ⁻¹	E (kJ/mol)	Ν	ΔT	$T_{\rm D24}$
this work	5.38×10^{16}	163.72	1.03	67.11	106.19°C
Paper 1[6]	5.26×10 ¹⁶	163.21	1.03	89.18	-
Paper 2[14]	3.67×10^{15}	155.38	0.98	-	-
Paper 3[15]	7.6×10^{16}	163.76	1	-	-





C. Experimental Result

Table II shows the comparison of estimated parameters between this work using the whole experimental data and the corresponding parameter obtained by other authors. The reaction process should also follow the n-order kinetics model. It is obvious that the fitted values of E and k_0 are in good accordance with the reference results. The simulated curve and experimental profiles of temperature and temperature rise rate curve are compared which shown in Fig. 3 and Fig. 4, respectively.



Fig. 4. Temperature rise rate vs Temperature for 20% DTBP.

V. RESULT OF DIFFERENT PROPORTION DATA USING CDPSO

A. Different Proportion Data of Adiabatic Temperature Rise

The kinetic parameters using different proportion of adiabatic temperature rise for 20% DTBP are summarized in Table III. Compared with the parameters calculated with the whole data, it is showed in Fig. 5-8 that only using no less than 90% proportion of experimental data, the kinetic parameters will be receivable. The kinetic parameters are not valid when the result was calculated by less than 90% especially the adiabatic temperature rise and the activation energy. When the data used in calculation is less than 50% proportion, the curves of temperature and temperature rise rate are obviously illogical.

TABLE III: COMPARISON OF THE KINETIC PARAMETERS USING DIFFERENT PROPORTION OF ADIABATIC TEMPERATURE RISE FOR 20% DTBP

Propor tion	Δ $T_{ad}(^{\circ}C)$	$k_0(s^{-1})$	E(kJ/mol)	п	$T_{\rm D24}(^{\circ}{\rm C})$	De_{TD24}
100%	67.11	38.52	163.72	1.03	106.19	-
90%	67.22	37.42	159.86	1.01	105.43	-0.71%
80%	76.72	43.08	178.87	1.85	106.84	0.61%
70%	77.44	46.16	189.15	2.15	107.68	1.40%
60%	72.93	44.27	182.69	1.79	107.22	0.97%
50%	83.60	46.04	188.84	2.47	107.46	1.19%
40%	70.65	42.23	175.95	1.48	106.84	0.61%
30%	51.33	35.78	154.05	0.32	105.53	-0.62%
20%	50.55	40.71	170.19	0.51	106.51	0.30%
10%	53.84	44.15	181.54	1.18	107.36	1.20%
9%	51.83	45.24	185.00	1.12	107.56	1.29%
8%	47.39	43.87	180.05	1.87	108.34	2.02%
7%	23.67	45.59	183.52	0.71	107.19	0.95%
6%	30.05	34.73	148.91	1.33	106.98	0.75%
5%	25.67	41.48	170.30	1.33	107.12	0.87%
4%	33.79	32.25	141.34	1.42	107.34	1.08%
3%	35.55	35.80	153.04	1.14	107.53	1.26%
2%	9.39	45.10	178.68	0.62	102.36	-3.61%
1%	13.25	45.45	180.77	1.75	97.29	-8.38%



Fig. 5. Temperature vs time of the kinetic parameters calculated by 60%-100% adiabatic temperature rise proportion data.



Fig. 6. Temperature vs time of the kinetic parameters calculated by 10%-50% adiabatic temperature rise proportion data.



Fig. 7. Temperature rise rate vs temperature of the kinetic parameters calculated by 60%-100% adiabatic temperature rise proportion data.



Fig. 8. Temperature rise rate vs temperature of the kinetic parameters calculated by 60%-100% adiabatic temperature rise proportion data.



Although it is difficult to get the accurate kinetic parameters using part of data, the value of T_{D24} is easier to obtain with CDPSO method. The deviation of T_{D24} is showed in Fig. 9 which is less than 2% using more than 9% data. Therefore, it is a good application to calculate T_{D24} by this method.

B. Different Proportion Data of Time

The kinetic parameters using different proportion of time for 20% DTBP are summarized in Table IV and Fig. 10-13. Compared with using adiabatic temperature rise proportion, the result of kinetic parameters using time proportion is worse. The deviation of kinetic parameters calculated by less than 90% data is non-neglectful. The curves of time vs temperature seem to be well-deviated with the experimental data but temperature vs temperature rise rate is awful using less than 90% data and the kinetic parameters are also away from true value.

The deviation of T_{D24} using part time proportion data is showed in Fig. 14. In accordance with the result of different adiabatic temperature rise proportion data, T_{D24} is well-deviated using this method. the value of T_{D24} is valid when the proportion of time data more than 30%. It proves the validity of T_{D24} calculation using this method again.

TABLE IV: COMPARISON OF THE KINETIC PARAMETERS USING DIFFERENT PROPORTION OF TIME FOR 20% DTBP

Proportion	$\Delta T_{ad}(^{\circ}C)$	$k_0(s^{-1})$	E(kJ/mol)	п	$T_{D24}(^{\circ}C)$	De_{TD24}
100%	67.11	38.52	163.72	1.03	106.19	-
90%	73.98	40.83	171.52	1.41	106.57	0.36%
80%	59.28	39.51	166.69	0.72	106.36	0.16%
70%	28.53	45.86	185.09	0.43	106.95	0.72%
60%	45.13	43.10	177.53	0.76	107.00	0.76%
50%	39.28	43.05	176.90	0.92	107.35	1.09%
40%	42.74	43.16	177.67	0.74	107.26	1.01%
30%	42.56	33.68	146.78	1.33	107.90	1.61%
20%	22.71	34.16	146.19	1.36	104.90	-1.22%
10%	17.63	42.60	172.53	1.79	102.24	-3.72%
9%	15.90	40.86	166.56	1.79	98.98	-6.79%
8%	19.41	32.44	139.97	1.94	96.27	-9.34%
7%	17.80	36.28	152.12	1.50	101.45	-4.46%
6%	15.19	42.92	173.05	1.58	101.11	-4.78%
5%	11.91	34.13	143.83	1.36	90.06	-15.19%
4%	7.48	32.92	138.42	0.81	87.40	-17.70%





Fig. 10. Temperature vs time of the kinetic parameters calculated by 60%-100% time proportion data.



Fig. 11. Temperature vs time of the kinetic parameters calculated by 10%-50% time proportion data.







Fig. 13. Temperature rise rate vs temperature of the kinetic parameters calculated by 10%-50% time proportion data.



Fig. 14. Deviation of T_{D24} using different proportion data of time.

C. Different Proportion Data of Temperature Rise Rate

The temperature rise rate curve was divided into a certain proportion which the curves before the maximum of temperature rise rate, the peak temperature, is 50%. Before the peak temperature, the curves were divided by different proportion of temperature rise rate. And after the peak temperature, the smaller temperature rise rate, the bigger proportion curves.

TABLE V: COMPARISON OF THE KINETIC PARAMETERS USING DIFFERENT PROPORTION OF TEMPERATURE RISE RATE FOR 20% DTBP

Proportion	$\Delta T_{ad}(^{\circ}C)$	$k_0(s^{-1})$	E(kJ/mol)	п	$T_{D24}(^{\circ}C)$	De_{TD24}
100%	67.11	38.52	163.72	1.03	106.19	-
90%	67.33	38.75	164.44	1.06	106.19	0.00
80%	67.52	39.23	166.07	1.09	106.37	0.17%
70%	67.22	37.65	160.66	1.02	105.56	-0.59%
60%	69.82	42.61	177.43	1.41	107.39	1.13%
50%	70.58	40.55	170.39	1.35	106.40	0.20%
40%	71.54	39.84	168.01	1.35	106.08	-0.11%
30%	60.59	33.17	145.52	0.54	104.05	-2.02%
20%	87.14	32.17	143.46	0.77	104.02	-2.05%
10%	63.96	46.07	188.19	1.67	107.50	1.23%
9%	70.33	33.55	147.67	0.44	104.96	-1.16%
8%	69.53	42.77	177.68	1.51	106.93	0.70%
7%	67.60	43.84	181.04	1.59	107.10	0.85%
6%	53.69	41.68	173.34	0.94	106.68	0.46%
5%	34.54	36.95	156.60	0.22	105.50	-0.65%
4%	68.54	38.87	165.06	0.82	106.30	0.10%
3%	58.02	40.44	169.65	0.74	106.52	0.31%
2%	53.74	40.22	168.82	0.44	106.41	0.21%
1%	49.98	40.69	170.09	0.84	107.09	0.84%



Fig. 15. Temperature vs time of the kinetic parameters calculated by 60%-100% temperature rise rate proportion data.



Fig. 16. Temperature vs time of the kinetic parameters calculated by 10%-50% temperature rise rate proportion data.



Fig. 17. Temperature rise rate vs temperature of the kinetic parameters calculated by 60%-100% temperature rise rate proportion data



Fig. 18. Temperature rise rate vs temperature of the kinetic parameters calculated by 10%-50% temperature rise rate proportion data.



Fig. 19. Deviation of T_{D24} using different proportion data of temperature rise rate.

This partition method is explicit to get the accurate proportion of known data if there has been the peak temperature rise rate in existence. The kinetic parameters using different proportion of temperature rise rate are summarized in Table V and Fig. 15-18 in which show the credible kinetic parameters are calculated by more than 70% data. the deviation of each parameters using more than 70% data is tiny.

The deviation of T_{D24} using part time proportion data is showed in Fig. 19. In accordance with the result of different adiabatic temperature rise and reaction time proportion data, T_{D24} is well-deviated using this method. the value of the deviation of T_{D24} is less than 2.05% using more than 1% data. It proves the validity of T_{D24} calculation using this method again.

VI. CONCLUSION

Conjugate direction particle swarm optimization (CDPSO) has the advantages of both the particle swarm optimization and the conjugate direction algorithm. It is an efficient and optimized algorithm which can deal with the calculation of kinetic parameters and T_{D24} from part experimental data.

Using the proportion data of temperature rise rate is better compared with adiabatic temperature rise or time proportion data at the same proportion. The valid kinetic parameters are obtained by no less than 70% proportion of temperature rise rate data.

The results of the three methods show that it is convenient and accurate to calculate T_{D24} using CDPSO algorithm using even 10% data.

CONFLICT OF INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

AUTHOR CONTRIBUTIONS

Xiao-Qiao Zhao conducted the research; Hao Wang compiled the programme; Wang-Hua Chen gave suggestions and comments; Xiao-Qiao Zhao and Wen-Qian Wu analyzed the data; Xiao-Qiao Zhao and Wen-Qian Wu wrote the paper; all authors had approved the final version.

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