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# Method of Selecting Active Parameters Using Sensitivity Analysis and Linear Programming

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## ABSTRACT

It is necessary to select appropriate active parameters to ensure both the accuracy and computation efficiency before the global analysis of chemical kinetic model. This paper proposes a new method for selecting the active parameters on the base of the combination of sensitivity analysis and linear programming. Compared with the usual methods for selecting active parameters, such as the local sensitive analysis, the characteristics of the proposed method is preliminary visualization of the possible influence of the selected active parameters on the model outputs in the process of parameter selection, ensuring the reliability of the selected active parameters. Considering the computation efficiency, the number of selected active parameters can be controlled in a suitable size through combining with dichotomy or other screening techniques. In the study, the pre-exponential factors of the Arrhenius equations in the USC-Mech II model were considered as the candidate parameters and the uncertainties of the pre-exponential factors were set. Taking the ignition of ethylene for example, the 10 reactions that can increase the ignition time of ethylene under a wide range of conditions with equivalence ratio of 1, 0.1 ~ 1 MPa and 1000 K ~ 1500 K were successfully selected using the proposed method. Then, the 10 active parameters were tested in each condition. The results showed that the selected active parameters can make the ignition delay time close to the target for each condition, which reflects the reliability of active parameter selection.

## ARTICLE HISTORY

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## KEYWORDS

Active parameter; sensitivity analysis; linear programming; selection method; chemical kinetic model

## Introduction

A chemical kinetic model typically consists of the thermodynamic and transport parameters of participating species and the parameterizing rate coefficients of reactions (Curran 2019). The reliability of the chemical kinetic model is determined by these parameters, which can be obtained from experimental databases, through theoretical calculations, analogies, or by educated guesses. However, the coupling of the uncertainty of these parameters and the nonlinearity in the chemical kinetic calculation may greatly reduce the reliability of existing chemical kinetic models, which results in obvious deviation compared with the experimental results, even if all of the parameters in the chemical kinetic model have less uncertainty (Frenklach, Wang, and Rabinowitz 1992).

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Generally, when one optimization method is executed, it is necessary to limit the number of the parameters involved in optimization for reducing the high-dimensionality problem of the chemical kinetic models and improving computational efficiency (Yang 2021). Therefore, a natural approach is to select parameters that have significant impacts on the model outputs to participate in optimization, and these parameters are called active parameters (Frenklach, Wang, and Rabinowitz 1992). There are many benefits in selecting appropriate active parameters. For example, it will be more efficient to use active parameters to construct a response surface (Tomlin et al. 2014). The obtained response surface can be applied to conduct further model analysis, such as global sensitivity analysis (Li, Yang, and Qi 2016; Russi et al. 2008), uncertainty quantification (Frenklach et al. 2016; Wang and Sheen 2015) and model optimization (Samu et al. 2017, 2018).

As a tool for evaluating the effects of parameter changes on the model, sensitivity analysis (Saltelli et al. 2005; Tomlin 2013; Turányi 1990, 1997) plays an important role in determining the active parameters in optimization. If the uncertainties of candidate parameters are small, the active parameters can be preliminarily selected from the candidate parameters according to the weight of sensitivity obtained by local sensitivity analysis. However, when the uncertainties of the candidate parameters are large, the variation of the parameters can deviate significantly from their nominal values, or there is a coupling relationship among the parameters, it may be scant to select the active parameters only by local sensitivity analysis (Tomlin 2013). There are many methods that can be used in conjunction with local sensitivity analysis to select the active parameters for increasing the reliability of selected active parameters. Their idea is to add additional constraints to the selection of active parameters. Such as, considering the uncertainties of the parameters and the number of degrees of freedom available for optimization (Frenklach 2007; Park et al. 2016; Sheen and Wang 2011; Xin et al. 2014; Yeates et al. 2015) and using optimization potential which can be measured by the product of the uncertainty and the parameter sensitivity (Cai and Pitsch 2014, 2015; Vom Lehn, Cai, and Pitsch 2019a, 2019b, 2020). The purpose of considering the uncertainties of the parameters and the number of degrees of freedom available for optimization is to ensure the number of active parameters and their uncertainty range meet the optimization requirements. In the work of Wang et al (Sheen and Wang 2011) 31 active parameters were selected based on these considerations. The reason for using optimization potential is that although a parameter has a great sensitivity, its uncertainty range is small, so the influence of the parameter change on the model is also limited. Therefore, in the active parameter selection, the comprehensive influence of parameter sensitivity and its uncertainty range should be considered. In the work of Cai et al (Cai and Pitsch 2015) they ranked the candidate parameters based on the optimization potential to select the appropriate active parameters. These methods have played a role in the related work, but there are still some difficulties in the selection of active parameters. For example, it is not clear how many active parameters to select will be effective for subsequent model analysis. If the influence of different number of active parameters on the model can be obtained before the model analysis, the model analysis can be carried out from a group of better active parameters, thus saving the time of model analysis and ensuring better analysis results. This paper is devoted to ensure the reliability and quantity adequacy of selected active parameters.

In this paper, a new method for selecting active parameters is proposed by combining local sensitivity analysis method and linear programming method (Megiddo 1987). Compared with the above-mentioned methods of selecting active parameters, the

characteristics of the proposed method is that preliminary visualization of the possible influence of the selected active parameters on the model outputs in the process of parameter selection, ensuring the reliability of the selected active parameters. It can help researchers determine the number of active parameters needed in relevant model analysis through further combining with dichotomy or other screening techniques. The rest of this paper includes an introduction to the mathematical principle of the proposed method, the instruction of the proposed method by the simulation of ignition of ethylene under a single condition, and an application case on the selection of active parameters for ignition of ethylene under wide conditions.

## Methodology

This section describes how the proposed method uses the local sensitivity analysis method to quantify the effects of multi-parameter changes on the output results of a chemical kinetic model, how to constrain the variation range of multiple parameters through linear programming, and how to iteratively select the active parameters.

### Local Sensitivity Analysis

Sensitivity analysis has an important role in chemical kinetics research, because it can determine the importance of relative parameters and helps in focusing on parameters with the greatest influence on predictions.

For the simplicity of mathematical description, consider a spatially homogeneous, dynamical system. And the change of vector  $\mathbf{Y}$  of the concentrations, mass fraction or other parameters over time can be calculated by solving the following initial value problem:

$$\frac{d\mathbf{Y}}{dt} = F(\mathbf{Y}, \boldsymbol{\alpha})\mathbf{Y}(t_0) = \mathbf{Y}_0 \quad (1)$$

The vector  $\boldsymbol{\alpha}$  may include rate coefficients, Arrhenius parameters, thermodynamic parameters, and so on;  $t_0$  is the initial time. The effect of a slight change  $\Delta\boldsymbol{\alpha}$  in the parameter set  $\boldsymbol{\alpha}$  on  $\mathbf{Y}$  at a given time can be calculated by the following Taylor expansion:

$$\mathbf{Y}(t, \boldsymbol{\alpha} + \Delta\boldsymbol{\alpha}) \approx \mathbf{Y}(t, \boldsymbol{\alpha}) + \frac{\partial \mathbf{Y}(t, \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} \Delta\boldsymbol{\alpha} \quad (2)$$

The first-order local sensitivity matrix  $s(t, \boldsymbol{\alpha})$  can be defined as  $\frac{\partial \mathbf{Y}(t, \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}}$ . For the convenience of calculation and evaluation,  $s(t, \boldsymbol{\alpha})$  is typically rewritten as the normalized form  $\mathbf{S}(t, \boldsymbol{\alpha})$ , where  $\mathbf{S}(t, \boldsymbol{\alpha}) = \frac{\partial \mathbf{Y}(t, \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} \frac{\boldsymbol{\alpha}}{\mathbf{Y}(t, \boldsymbol{\alpha})}$ . Then, Equation (3) can be derived from Equation (2), as follows:

$$\frac{\mathbf{Y}(t, \boldsymbol{\alpha} + \Delta\boldsymbol{\alpha}) - \mathbf{Y}(t, \boldsymbol{\alpha})}{\mathbf{Y}(t, \boldsymbol{\alpha})} \approx \frac{\partial \mathbf{Y}(t, \boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} \frac{\Delta\boldsymbol{\alpha}}{\mathbf{Y}(t, \boldsymbol{\alpha})} = \mathbf{S}(t, \boldsymbol{\alpha}) \frac{\Delta\boldsymbol{\alpha}}{\boldsymbol{\alpha}} \quad (3)$$

Equation (3) describes the influence of parameter perturbation on the relative change of the model output results. Then, considering the test value vector  $\mathbf{Y}_E$  and its corresponding time vector  $t_E$ , we expect the  $\mathbf{Y}(t_E, \boldsymbol{\alpha} + \Delta\boldsymbol{\alpha})$  will be closer to  $\mathbf{Y}_E$ . Under this condition,  $\Delta\boldsymbol{\alpha}$  is the variation of  $\boldsymbol{\alpha}$  in its uncertainty ranges at initial time  $t_0$ , which is typically not a miniscule change. The substitution of  $\mathbf{Y}_E$  for  $\mathbf{Y}(t, \boldsymbol{\alpha} + \Delta\boldsymbol{\alpha})$  will affect the mathematical properties of

Equation (3). However, by analogy, we can construct the form of the substitution and assume that the linear relationship still exists:

$$\frac{Y_E - Y(t_E, \alpha)}{Y(t_E, \alpha)} \bar{S}(t_E, \alpha) \frac{\Delta \alpha}{\alpha} \quad (4)$$

$$\bar{S}(t_E, \alpha) = \frac{1}{t_E - t_0} \int_{t_0}^{t_E} S(t, \alpha) dt \quad (5)$$

Where  $\bar{S}(t_E, \alpha)$  represents the characteristic sensitivity matrix corresponding to each time point from the initial  $t_0$  to  $t_E$ , and the absolute values of its components are used to evaluate the disturbance ability of the parameter changes on the calculated results of this time interval. With a larger absolute value, the disturbance ability becomes stronger. The relationship expressed in (4) is the carrier of the linear programming implementation.

### Linear Programming

Linear programming (LP) is defined as the problem of maximizing or minimizing a linear function that is subjected to linear constraints. Denote the column vector  $\mathbf{X} = \frac{\Delta \alpha}{\alpha}$ , the matrix  $\mathbf{A} = \bar{S}(t_E, \alpha)$  and the column vector  $\mathbf{B} = \frac{Y_E - Y(t_E, \alpha)}{Y(t_E, \alpha)}$ . For selecting active parameters, it is generally expected that fewer parameters require adjustment to achieve the optimization purpose; therefore, the following objective function is constructed and its minimum value is sought:

$$f = \sum |\mathbf{X}| \quad (6)$$

Nonlinear function (6) represents the sum of the absolute values of the components of  $\mathbf{X}$ , where the components whose value is not zero are taken as the active parameter.

From the relationship in (4), the inequality constraints can be constructed as follows:

$$\begin{cases} A_i \mathbf{X} \geq z B_i B_i \geq 0 \\ A_i \mathbf{X} < z B_i B_i < 0 \end{cases} \quad (7)$$

Here,  $A_i$  is the row vector composed of the  $i^{\text{th}}$  row elements of matrix  $\mathbf{A}$ ,  $B_i \in \mathbf{B}$  and  $z$  is the reduction factor whose initial value is 1.

If the coupling relationship among some candidate parameters can be expressed by linear relationship, additional equality constraints can be constructed as follows:

$$X_{j0} = \beta_0 + \beta_1 X_{j1} + \beta_2 X_{j2} + \beta_3 X_{j3} + \dots + \beta_n X_{jn} \quad (8)$$

Here,  $X_{jN} \in X$  and  $\beta_N$  is non-zero coefficient where  $N = 0, 1, 2, \dots, n$ . The most intuitive interpretation of equality constraint (11) is that when a candidate parameter is selected as an active parameter, the candidate parameter coupled with it may also be selected as an active parameter.

Because  $\Delta \alpha$  varies in its uncertainty ranges,  $X$  naturally has the following boundaries:

$$\mathbf{X}_{min} \leq \mathbf{X} \leq \mathbf{X}_{max} \quad (9)$$

Where  $\mathbf{X}_{min}$  and  $\mathbf{X}_{max}$  is the lower bound and upper on the uncertainty range of  $\mathbf{X}$ , respectively.

Linear programming requires its objective function to be linear, so the nonlinear Equation (6) must be transformed into one linear form.  $U$  and  $V$  are the two intermediate quantities to represent  $X$  and  $|X|$ . The alternative forms constructed are shown in Equation (11) and Equation (12). Here, the vectors  $U$  and  $V$  are introduced into function (6), and the following linear function is obtained:

$$f = \sum(U + V) \quad (10)$$

The transformation from function (6) to function (10) requires two additional equality constraints and two inequality constraints as follows:

$$X = U - V \quad (11)$$

$$|X| = U + V \quad (12)$$

$$U = \frac{|X|+X}{2} \rightarrow U \geq 0 \quad (13)$$

$$V = \frac{|X|-X}{2} \rightarrow V \geq 0 \quad (14)$$

Finally, Equations (7–14) constitute a complete linear programming problem. In this linear programming problem, it almost always has a solution by reducing the value of  $z$ .

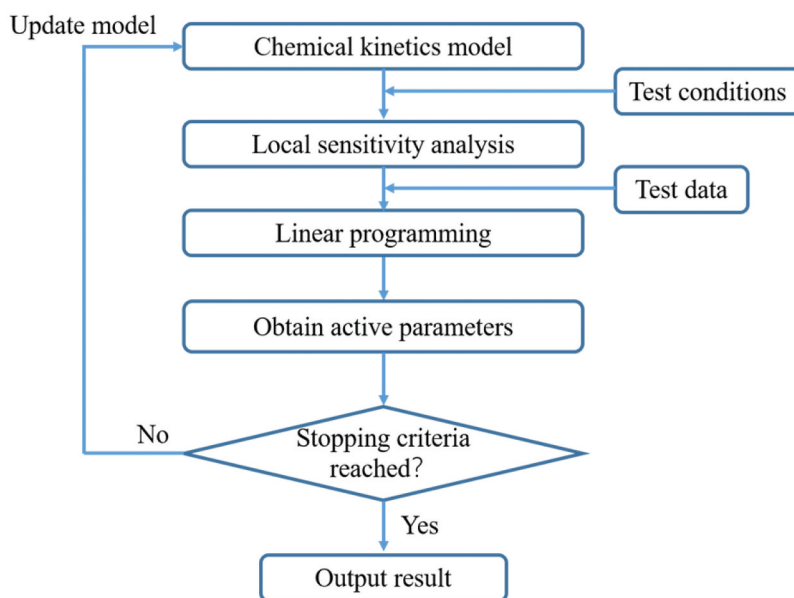
So far, the establishment process of the proposed method and the process of selecting active parameters have been introduced, and considered the problem of how to determine the active parameters when there is a coupling relationship among candidate parameters to a certain extent. However, there are still other problems need attention. First, when the uncertainty range of candidate parameters is large, the local sensitivity analysis method has defects. Second, it is unable to intuitively judge whether the selected active parameters are effective. To solve these problems, the iterative procedures will be introduced.

### Iterative Procedures

Linear programming is used after local sensitivity analysis of candidate parameters. Sensitivity analysis data and linear constraints are used to select a group of active parameters from the candidate parameters and obtain the adjustment values of this group of active parameters. The iterative procedures repeat the above steps. Obviously, after kinetic model is updated, the influence of the selected active parameters on the kinetic model can be directly observed. It is one purpose of using the iterative procedures. The active parameters selected in a single iteration are not sufficient, and their influence on the model is difficult to approach the expectation. Therefore, another purpose of using iterative procedures is to select enough active parameters so that their influence on the model is close to or equal to the expectation.

The initial set of  $\alpha$  is denoted by  $\alpha_0$  and its solution set is  $\Delta\alpha_0$ . Denote  $\alpha_1 = \alpha_0 + \Delta\alpha_0$ ; then, we need to obtain the solution set  $\Delta\alpha_1$ . By analogy, for the  $n^{\text{th}}$  iteration, the relationship in (4) is updated as follows:

$$B_{n-1} = \frac{Y_E - Y(t_E, \alpha_{n-1})}{Y(t_E, \alpha_{n-1})} \sim \bar{S}(t_E, \alpha_{n-1}) \frac{\Delta\alpha_{n-1}}{\alpha_{n-1}} = \bar{S}(t_E, \alpha_{n-1}) X_{n-1} \quad (15)$$



**Figure 1.** The schematic of the iteration procedures.

Then, by using Equation (15), Equations (7) ~ (14) are updated and solved to obtain  $\Delta\alpha_{n-1}$ . The variation range of  $\mathbf{X}_{n-1}$  is always within  $[\mathbf{X}_{n-1,min}, \mathbf{X}_{n-1,max}]$ . The stopping criteria can be set according to requirements such as the maximum number of iterations or the change of the parameters in two adjacent iterations and so on.

In each iteration, appropriate candidate parameters will be selected as active parameters and the changes of active parameters in the chemical kinetic model will be updated in time. Therefore, the selection of active parameters and the influence of their value changes on the model can be directly observed, which ensures the effectiveness of the selection of active parameters. A graphical representation of the iteration procedures is shown in Figure 1:

## Instructions of Method

In this section, the ignition delay time of premixed ethylene and oxygen was simulated under certain conditions in the constant volume adiabatic reactor model of Cantera (Goodwin et al. 2022). The pre-exponential factors of the Arrhenius equations in the USC-Mech II model (Wang et al. 2007) were considered as candidate parameters. Then, the proposed method was used to select the active parameters related to the ignition delay time. The results confirm the feasibility of the proposed method.

## Case Study

The USC-Mech II model is a chemical kinetic model that considers the H<sub>2</sub>/CO/C<sub>1</sub>-C<sub>4</sub> combustion developed by Wang et al (Wang et al. 2007). The model comprises 111 species and 784 reactions, and has many applications in combustion simulation (El Merhubi et al. 2016; Wang et al. 2017; Zhang et al. 2012). This case study used the USC-Mech II model to

simulate the ignition delay time of a mixture of ethylene ( $C_2H_4$ ) and oxygen ( $O_2$ ) in the constant volume adiabatic reactor model of Cantera (Goodwin et al. 2022) under 1400 K and 0.1 MPa. It is worth noting that the set values of temperature and pressure are only the values at initial time, and their values will change over time in the simulation. The initial mole fraction of ethylene and oxygen in the mixture is 0.25 and 0.75, respectively, so the equivalence ratio is 1. In this work, the time period from the initial time until the concentration of OH reaches its peak is defined as the ignition delay time. Under the above simulation conditions, the variation of OH mole fraction is shown in the following figure:

Figure 2 shows that the ignition delay time calculated by USC-Mech II model is 0.064 ms under the conditions of 1400 K, 0.1 MPa, constant volume and the equivalence ratio of  $C_2H_4$  and  $O_2$  is 1. Now consider a question: if the uncertainty range of ignition delay time at this condition is  $\pm 25\%$ , namely 0.048 ms to 0.080 ms and the pre-exponential factors of the model are taken as the candidate parameters, how should the active parameters be selected?

### Procedures of the Proposed Method

The procedures for the proposed method to select active parameters from the candidate parameters are introduced as follows:

- (1) The first step is to determine the local sensitivity analysis object. The derivative of OH mole fraction with respect to time is selected as the local sensitivity analysis object to characterize the ignition delay time. Because the derivative at the peak of the OH mole fraction is constant zero, the ignition delay time can be determined by the time when the derivative is zero.

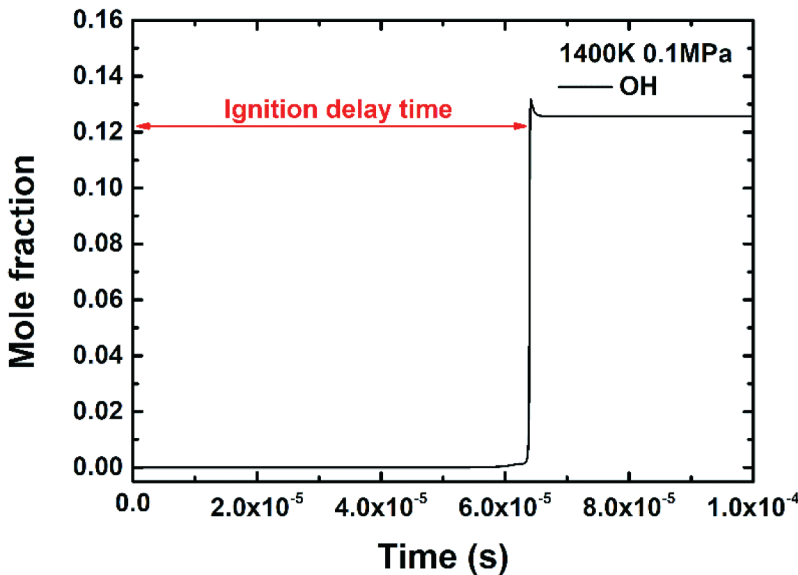


Figure 2. Variation of OH mole fraction of the reaction  $C_2H_4 + O_2$  in the initial conditions of 1400 K, 0.1 MPa and constant volume.



- (2) The second step is to assume the uncertainty factor  $u$  of the candidate parameters. Considering that the nominal value of the candidate parameter is  $A_0$ , the lower bound of the uncertainty range is  $A_{min}$ , and the upper bound of the uncertainty range is  $A_{max}$ , then the uncertainty factor  $u$  is represented by the following formula (Baulch et al. 2005):

$$u = \log_{10} \left( \frac{A_0}{A_{min}} \right) = \log_{10} \left( \frac{A_{max}}{A_0} \right) \quad (16)$$

Here, the value of  $u$  is assumed to be 0.3, that is, the uncertainty range of the pre-exponential factor is  $0.5A_0 \sim 2A_0$ .

- (3) The third step is to analyze the local sensitivity of the selected object and select the active parameters with linear programming. After the local sensitivity analysis of the derivative of OH mole fraction with respect to time has been calculated, the active parameters can be selected by linear programming according to the uncertainty range of ignition delay time. It is known that the upper bound of the uncertainty range of the ignition delay time is 0.080 ms, the following formula can be obtained from the previous section:

$$B = \frac{Y_E - Y(t_E, \alpha)}{Y(t_E, \alpha)} = \frac{\frac{dOH}{dt}_{E, t=0.08} - \frac{dOH}{dt}(0.08, \alpha)}{\frac{dOH}{dt}(0.08, \alpha)} \quad (17)$$

$$A = \bar{S}(t_E, \alpha) = \frac{1}{t_E - t_0} \int_{t_0}^{t_E} S(t, \alpha) dt = \frac{1}{0.08} \int_0^{0.08} S(t, \alpha) dt \quad (18)$$

When the derivative of OH mole fraction with respect to time is 0 at 0.080 ms, it represents the peak there, but using linear programming requires some additional processing when  $\frac{dOH}{dt}_{E, t=0.08}$  is 0. Here we characterize the peak with a very larger derivative value, that is, let  $\frac{dOH}{dt}_{E, t=0.08} = 10^4$  rather than  $\frac{dOH}{dt}_{E, t=0.08} = 0$ . Based on the upper and lower bounds of uncertainty range of ignition delay time, the active parameters are selected by linear programming respectively.

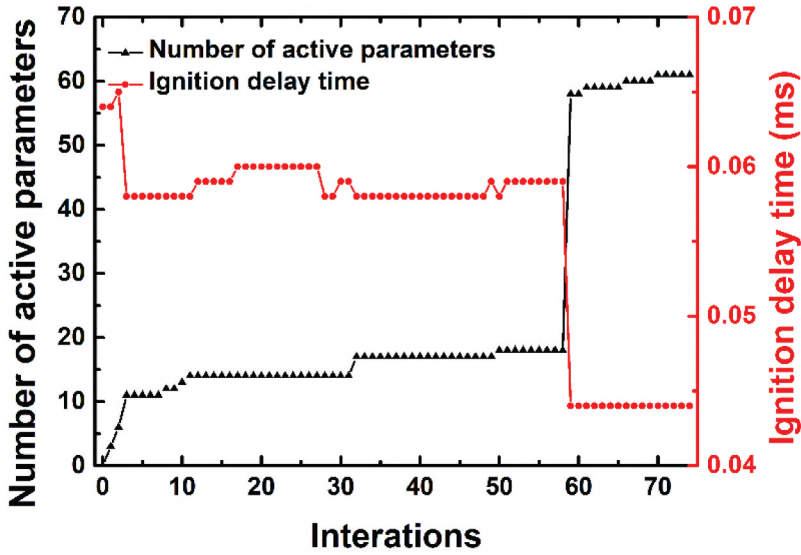
- (4) In each iteration, the variation of the pre-exponential factors does not exceed their uncertainty range. The termination condition of the iteration is set as the calculated ignition delay time is less than 0.05 ms or more than 0.075 ms.

## Results and Discussions

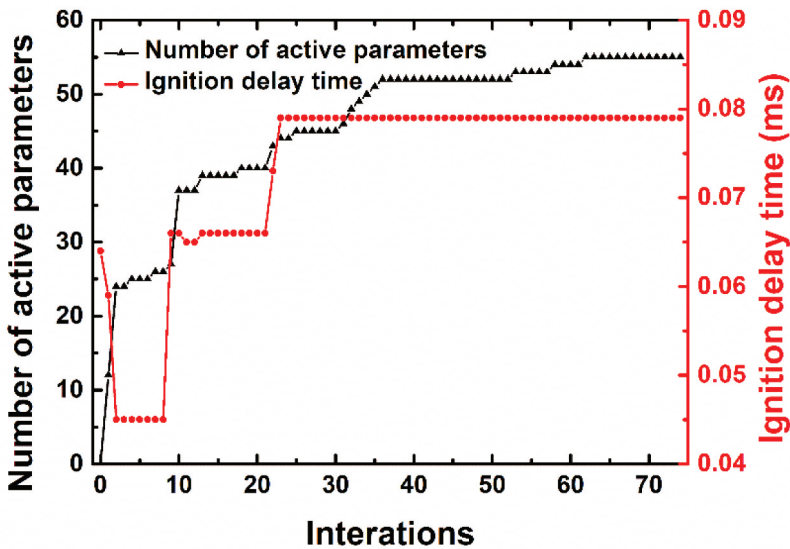
Figure 3 and Figure 4 show the results of selecting active parameters for the lower and upper bounds of the uncertainty range of ignition delay time respectively.

As can be seen from the two figures:

- (1) The number of the selected active parameters increases with iterations, and their overall impacts on the ignition delay time can be observed during each iteration. The active parameters selected by the proposed method can change the ignition delay time in the desired direction.
- (2) In Figure 3, when the number of the selected active parameters reaches 11, the ignition delay time of the model decreases to 0.058 ms, but then from the 4<sup>th</sup> iteration to the 58<sup>th</sup> iteration, the number of active parameters only increases from 11 to 18,



**Figure 3.** Variation of number of the selected active parameters for the lower bound of the uncertainty range of ignition delay time under the case setting conditions.



**Figure 4.** Variation of number of the selected active parameters for the upper bound of the uncertainty range of ignition delay time under the case setting conditions.

and the ignition delay time does not change significantly. However, at the 59<sup>th</sup> iteration, the number of selected active parameters jumps from 18 to 58, and the ignition delay time drops to 0.044 ms, which meets the termination condition of selection. This jump occurs because the number of active parameters satisfying the constraints sharply increased in the 59<sup>th</sup> iteration.

- (3) In [Figure 4](#), an important incident is found, although it is an accidental situation caused by our algorithm. In the second iteration, it can be found that the ignition delay time decreases from 0.064 ms to 0.045 ms, and the number of the selected active parameters is 24, while the number of active parameters selected to reach this ignition delay time in [Figure 3](#) is 58. By comparison, only one active parameter is the same in these two active parameter sets. This directly indicates that the selection of active parameters with the same influence on ignition delay time can be different under the same conditions, which is also applicable to other research objects. The most important thing is to ensure the validity of the selected active parameters. At the 23<sup>rd</sup> iteration, the number of selected active parameters is 44, and the ignition delay time rises to 0.079 ms, which meets the selection requirements of active parameters.

[Figure 3](#) and [Figure 4](#) present that the selected active parameters are able to be evaluated by the proposed method. However, in model analysis, especially global sensitivity analysis or global uncertainty analysis, in order to improve the calculation efficiency, it is necessary to limit the number of the active parameters used.

Next, the selected active parameters will be further screened. Here, the results in [Figure 4](#) are taken as an example. When the iteration terminates, 44 active parameters are selected after 23 iterations. In order to further screen these active parameters, the weight  $w$  is introduced to evaluate the importance of active parameters as follows:

$$w_i = \frac{N}{\sum_{j=1}^N F_{ij}} \quad (19)$$

Where  $w_i$  represents the weight of an active parameter,  $F_{ij}$  represents the rank of the absolute value of the characteristic sensitivity  $\bar{S}_i$  of this active parameter at the  $j^{\text{th}}$  iteration, and when the rank of  $\bar{S}_i$  is 1, the absolute value of its characteristic sensitivity is the largest, and  $N$  represents the total number of iterations.

The larger  $w$  of the active parameter is, the more important the active parameter is, although it may not be completely accurate. The active parameters are further screened by dichotomy. Although the dichotomy is not the optimal method for screening active parameters, its screening efficiency is high and its mathematical essence is easy to understand, which is the reason for choosing it in this paper. According to the weight ranking, the active parameters will be divided into two groups of similar size in order, that is, the active parameters ranked 1–22 form one group A, and the active parameters ranked 23–44 form another group B. Here, the values of the active parameters at the 23<sup>rd</sup> iteration are taken as the reference values, and the influence of group A and group B on the ignition delay time of the model is compared. The group which is closer to the ignition delay time of 0.08 ms will be selected and divided again, and the above steps will be repeated. The screened results are shown in [Figure 5](#) below:

From [Figure 5](#), it can be found that the active parameters that have important impacts on the ignition delay time can be further screened based on the weight ranking and dichotomy. However, if the active parameters are selected only through the weight ranking, there may be a deficiency. In [Figure 5](#), the group of the top five active parameters in the weight ranking is far less influential on the ignition delay time than the group of the active parameters with weight ranking 6 ~ 11. The following table shows the reactions and the multiplication factors of their pre-exponential factors corresponding to weight ranking from 1 to 11:

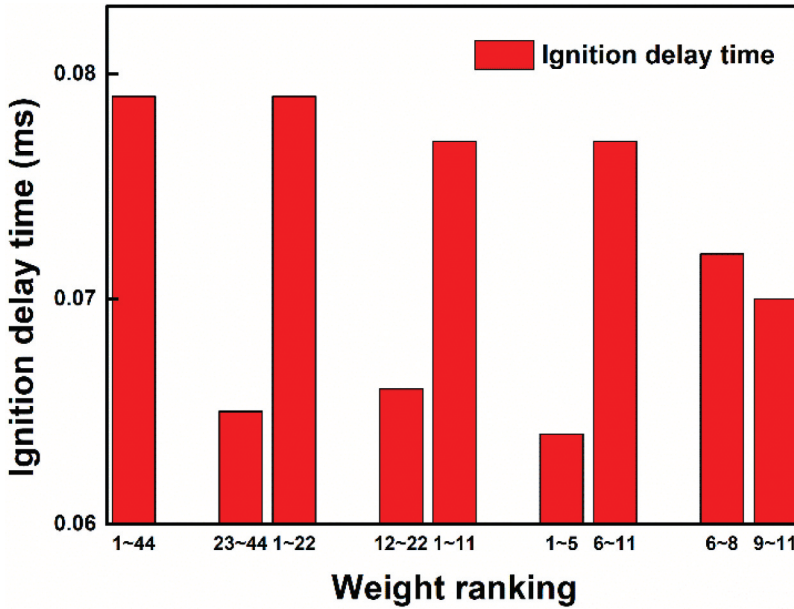


Figure 5. Influence of different groups of active parameters on ignition delay time.

Table 1. The reactions and the multiplication factors of their pre-exponential factors corresponding to weight ranking of Figure 5.

No.	Reaction	Weight ranking	Multiplication factor
16	$H + HO_2 \rightleftharpoons 2 OH$	1	2.00
125	$CH_4 + OH \rightleftharpoons CH_3 + H_2O$	2	0.50
779	$O_2 + c-C_4H_5 \rightleftharpoons CH_2CHO + CH_2CO$	3	0.50
48	$CH + H_2 \rightleftharpoons CH_2 + H$	4	0.50
49	$CH + H_2O \rightleftharpoons CH_2O + H$	5	2.00
41	$HCO + O_2 \rightleftharpoons CO + HO_2$	6	1.51
17	$HO_2 + O \rightleftharpoons O_2 + OH$	7	0.50
68	$CH_2^* + H \rightleftharpoons CH + H_2$	8	0.97
96	$CH_3 + HO_2 \rightleftharpoons CH_3O + OH$	9	0.50
126	$CH + CH_4 \rightleftharpoons C_2H_4 + H$	10	0.50
52	$CH + CO_2 \rightleftharpoons CO + HCO$	11	0.50

In Table 1, although the adjustment values of the top five active parameters according to weight ranking are large, the high local sensitivity weight of active parameters does not necessarily mean that adjusting their parameters will have great impacts on the model, which indicates that it may be insufficient to select active parameters only by local sensitivity analysis method. The method proposed in this paper avoids this shortcoming and can ensure the reliability of active parameter selection.

## Application

In order to exclude the distinctiveness of the above case, this section further demonstrates the feasibility of the proposed method for selecting the active parameters under a wide range of conditions. It also takes the ignition delay time of ethylene as the research object.

## Simulation Settings

Based on the previous section, the ignition delay time of ethylene were calculated under different conditions when the equivalence ratio was 1, and the ignition delay time was increased by 1.25 times as the test time set  $t_E$  used in the proposed method, and the test value corresponding to each time point in the test time set was 10,000, as shown in Table 2. The termination condition is that a group of active parameters is found, which increases the ignition delay time under all operating conditions. The other settings are the same as in the previous section.

Under the setting conditions in Table 2, the proposed method is used to select a group of active parameters that increase the ignition delay time under wide conditions. Although no active parameters that increased the ignition delay time (IDT) by 1.25 times were observed in subsequent work, the selected active parameters also make the ignition delay time of each working condition close to the target.

## Results and Discussions

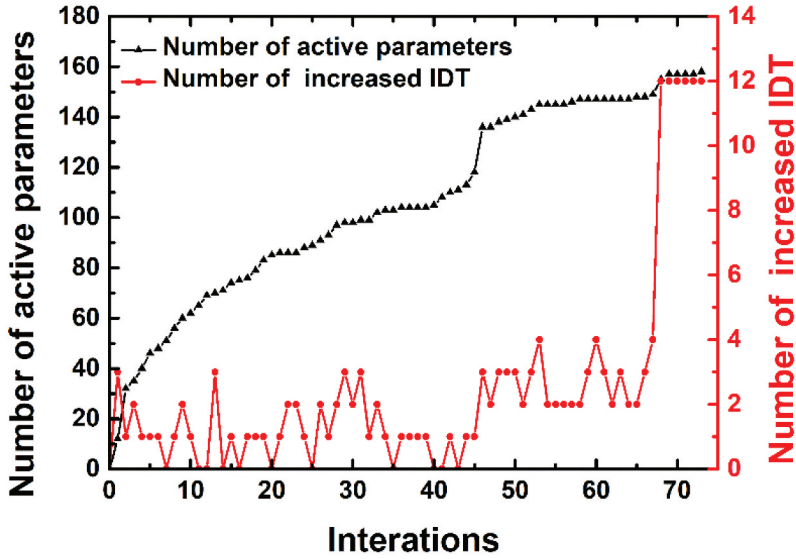
Figure 6 shows the results of using the proposed method to select the active parameters that increase the ignition delay time of each condition. It can be seen from Figure 6 that in the 68<sup>th</sup> iteration, the proposed method found a group of active parameters that increase the ignition delay time under all conditions, which verifies the feasibility of the proposed method under multiple conditions. But the number of active parameters selected is 155 and needs further be reduced.

In the previous section, Equation (19) was used to calculate the weight of each active parameter under a single condition. Here, the weight of each active parameter under multiple conditions is the sum of the weight of each condition. After ranking the active parameters based on their weights, the dichotomy was used to screen the active parameters. The following Table 3 shows the selected active parameters that meet the requirements after screening and the corresponding increase of ignition delay time. Based on the data in Tables 3, 4 shows the reactions corresponding to the active parameters with weight ranking 58 ~ 67 and the multiplication factors of their pre-exponential factors.

To further verify the reliability of the active parameters selected in Table 4, the variation of ignition delay time under each condition in Table 2 were studied when only pre-

**Table 2.** Ignition delay time of ethylene under wide conditions and test setting in the process of active parameter selection.

No.	Pressure, MPa	Temperature, K	IDT, ms	$t_E$ (IDT*1.25), ms	$Y_E (\frac{dOH}{dt}_{E,t_E})$
1	0.1	1000	5.95	7.44	10000
2		1100	1.57	1.97	
3		1200	4.82E-01	6.03E-01	
4		1300	1.62E-01	2.03E-01	
5		1400	6.40E-02	8.00E-02	
6		1500	2.77E-02	3.46E-02	
7	1	1000	7.50E-01	9.37E-01	
8		1100	2.10E-01	2.62E-01	
9		1200	7.28E-02	9.10E-02	
10		1300	2.79E-02	3.49E-02	
11		1400	1.09E-02	1.37E-02	
12		1500	4.48E-03	5.60E-03	



**Figure 6.** Variation of number of the selected active parameters and increased IDT under conditions of Table 2.

**Table 3.** The groups of selected active parameters according to weigh ranking and the corresponded increase percent of the ignition delay time.

Weight ranking	Maximum increase	Minimum increase	Mean increase
1~155	39%	5%	14%
1~77	30%	10%	16%
39~77	59%	8%	21%
58~77	48%	8%	20%
58~67	32%	8%	14%
63~67	51%	6%	11%

**Table 4.** The reactions and the multiplication factors of their pre-exponential factors corresponding to weight ranking of Table 3.

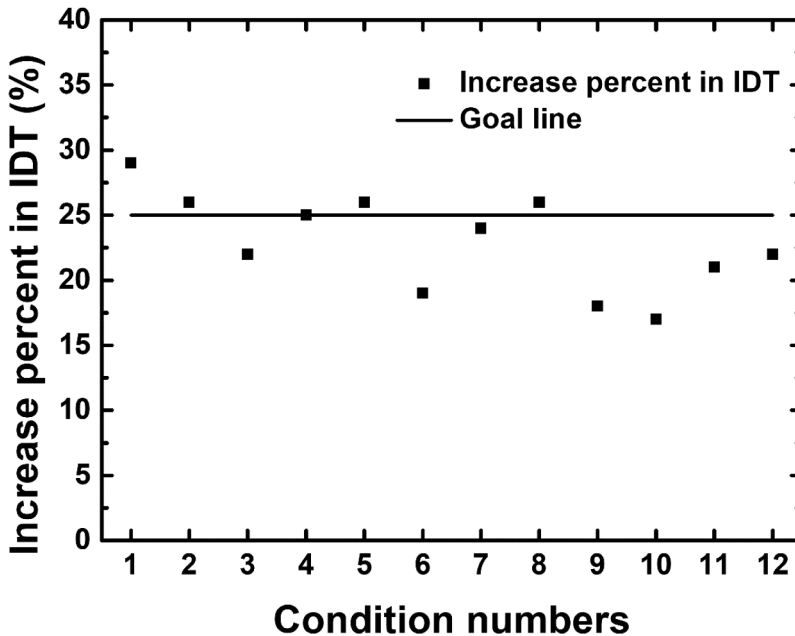
No.	Reaction	Weight ranking	Multiplication factor
1	$H + O_2 \rightleftharpoons O + OH$	58	1.00
41	$HCO + O_2 \rightleftharpoons CO + HO_2$	59	2.00
125	$CH_4 + OH \rightleftharpoons CH_3 + H_2O$	60	1.45
615	$H + tC_4H_9 \rightleftharpoons CH_3 + iC_3H_7$	61	0.50
24	$HO_2 + OH \rightleftharpoons H_2O + O_2$	62	0.95
704	$H + HOC_6H_4CH_3 \rightleftharpoons C_6H_5CH_3 + OH$	63	2.00
96	$CH_3 + HO_2 \rightleftharpoons CH_3O + OH$	64	0.50
87	$CH + CH_2O \rightleftharpoons CH_2CO + H$	65	0.50
708	$C_6H_6 + OH \rightleftharpoons C_6H_5 + H_2O$	66	2.00
86	$CH_2O + HO_2 \rightleftharpoons H_2O_2 + HCO$	67	0.78

**Table 5.** The values of the selected active parameters when the increase in ignition delay time is close to 25% under different conditions (1).

No. (Reaction)	Multiplication factor					
	Condition 1	Condition 2	Condition 3	Condition 4	Condition 5	Condition 6
1	1.00	1.52	0.50	0.50	1.00	1.00
24	0.95	1.19	0.74	2.00	0.95	0.95
41	2.00	1.57	1.34	1.25	2.00	1.38
86	0.78	1.53	0.78	0.78	0.78	0.78
87	0.50	1.58	0.50	0.75	0.50	0.50
96	0.50	0.50	0.50	0.50	0.50	0.52
125	1.45	1.45	0.50	1.50	1.45	1.45
615	0.56	1.98	1.81	0.57	0.50	0.50
704	1.71	0.69	0.54	0.50	2.00	2.00
708	2.00	1.29	0.87	1.90	2.00	2.00
Increase percent in IDT	29%	26%	22%	25%	26%	19%

**Table 6.** The values of the selected active parameters when the increase in ignition delay time is close to 25% under different conditions (2).

No. (Reaction)	Multiplication factor					
	Condition 7	Condition 8	Condition 9	Condition 10	Condition 11	Condition 12
1	1.00	1.00	2.00	0.50	0.50	1.00
24	1.32	0.94	2.00	2.00	0.50	0.95
41	2.00	2.00	0.50	1.58	0.94	2.00
86	1.61	0.78	0.50	0.50	0.500	0.78
87	2.00	0.50	0.50	0.50	0.50	0.50
96	0.50	0.50	1.50	0.50	0.53	0.50
125	1.45	1.45	2.00	2.00	1.34	1.45
615	0.88	0.50	2.00	2.00	0.50	0.50
704	0.50	2.00	0.53	0.50	0.72	2.00
708	2.00	2.00	2.00	2.00	0.53	2.00
Increase percent in IDT	24%	26%	18%	17%	21%	22%

**Figure 7.** Increase percent in ignition delay time under different conditions according to Tables 5 and 6.

exponential factors were considered as candidate parameters of the 10 reactions in Table 4. The termination condition of the iteration was set as the number of iterations is more than 200 to observe the effect of the selected parameters. Tables 5 and 6 show the values of the selected active parameters when the increase percent in ignition delay time is close to 25% under different conditions. Figure 7 shows the effects of the selection of active parameters in Tables 5 and 6 on the increase in ignition delay time. From Figure 7, it can be found that the selected active parameters can better approach the target for each condition, which reflects the reliability of active parameter selection.

## Concluding Remarks

Based on sensitivity analysis and linear programming, this paper proposes a new method for selecting the active parameters. Compared with the other methods for selecting active parameters, the characteristics of the proposed method is that preliminarily visualizing the influence of the selected active parameters on the model outputs to make sure the reliability of the selected active parameters. In Section 3 and Section 4, the reliability and characteristics of the proposed method were demonstrated by selecting the active parameters related to ignition delay time of ethylene under a wide range of conditions.

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## Disclosure statement

No potential conflict of interest was reported by the author(s).

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