

# Computational aspects of Simplification of Mathematical Models of Chemical Reaction Systems

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**Abstract.** The primary objective of this study is to develop a procedure for simplifying the mathematical model of a chemical reaction by reducing the number of steps and species in the reaction scheme. The procedure is based on the sensitivity analysis of the model functional to the change in the model parameters. The application of this procedure makes it possible to accelerate and improve the construction of mathematical models for chemical reactions, as this does not require the calculation of sensitivity coefficients at various time points or sensitivity matrix analysis. The efficiency of using this procedure was demonstrated by comparative results of modeling of formaldehyde oxidation in terms of detailed and reduced schemes. Computational aspects of the solution of the problems of chemical kinetics by the global sensitivity method using the example of the formaldehyde oxidation reaction are presented.

## 1. Introduction

The problem of parameter identification of the reaction kinetic model has an important scientific and practical significance and is relevant at the present time [1]. The mathematical model of any chemical reaction is characterized by a certain set of parameters that can be determined by a certain error due to inaccurate measurements, the lack of a sufficient number of experimental data, an incomplete understanding of the reaction mechanism, and so on. Thus, the problem of parameter determination of kinetic model has a number of solutions.

The Authors of this work are developing a numerical approach for analyzing the parametric identifiability of the model, which includes criteria for model identification, as well as procedures for excluding the non-identifiability and reduction of the kinetic model [2]. Identifiability is understood as the possibility to determine the model parameters with a given accuracy. It is necessary to identify the model parameters that most influence the description of the process. This brings about the problem that is aimed at reducing the dimensionality of the model by eliminating the little influencing parameters, i.e. the problem of reducing the model [3, 4]. Moreover, very large mechanisms cannot be introduced into complex multi-dimensional computational fluid dynamics codes for the modeling of the combustion of practical fuels. For this reason, efforts are being made to employ reduction techniques for the simplification of large mechanisms in order to keep the essential features of the chemistry in realistic combustor configurations.

Researchers have proposed many methods for reducing kinetic models. Among them, the first methods, which refer to time scale separation methods, and which have not lost their relevance, and modern methods such as the directed relation graphs method (the method targets, first of all, exclusion of species) and the sensitivity analysis methods [5, 6]. In recent years, sensitivity analysis of numerical models has gained wide use, which is associated with the advancement of computer technology and computer modeling [7, 8]. Analysis of sensitivity of a kinetic model to the variation of rate constants for single steps or the whole set of steps makes it possible to evaluate how much the function depends on the variation of a particular parameter and which parameters are crucial for the model and which have little influence on the solution when vary [8, 9, 10, 11, 12] and provides additional information about the model, being able to serve for verification.

This paper proposes a procedure for simplifying the mathematical model of a chemical reaction by reducing the number of steps and species in the reaction scheme, which is based on the sensitivity analysis of the model functional to the change in the model parameters. The model functional includes summation over the reaction substances, several temperatures, and several time points. This is the way to obtain a reduced scheme consistent with the detailed scheme for the specified range of conditions.

Computational aspects of the solution of the problems of chemical kinetics by the global sensitivity method using the example of the formaldehyde oxidation reaction are presented. The results of comparison of local, global and total global sensitivity coefficients are shown.

## 2. Mathematical model

Chemical kinetic equations composed for the description of the hydrogen oxidation reaction represent a system of ordinary nonlinear differential equations for a model of isothermal non-stationary reaction not accompanied by a change in the volume of the reaction mixture, occurring in a closed system according to the law of mass action [13, 14]:

$$\frac{dx_i}{dt} = \sum_{j=1}^N B_{ij}(k_j \prod_{i=1}^M (x_i)^{|\alpha_{ij}|} - k_{-j} \prod_{i=1}^M (x_i)^{\beta_{ij}}), i = 1, \dots, M, \quad (1)$$

the initial conditions being as follows:  $x_i(0) = x_i^0$ .

Here  $x_i$  are concentrations of the substances,  $M$  is the number of substances,  $N$  is the number of steps,  $B_{ij}$  are stoichiometric coefficients,  $\alpha_{ij}$  are negative elements of  $B_{ij}$ ,  $\beta_{ij}$  are positive elements of  $B_{ij}$ ,  $w_j$  is the rate of the  $j$ -th step,  $k_j$ ,  $k_{-j}$  are the rate constants for the forward and reverse reaction, respectively,  $t$  is time.

The rate constants for reactions were calculated from the Arrhenius equation:

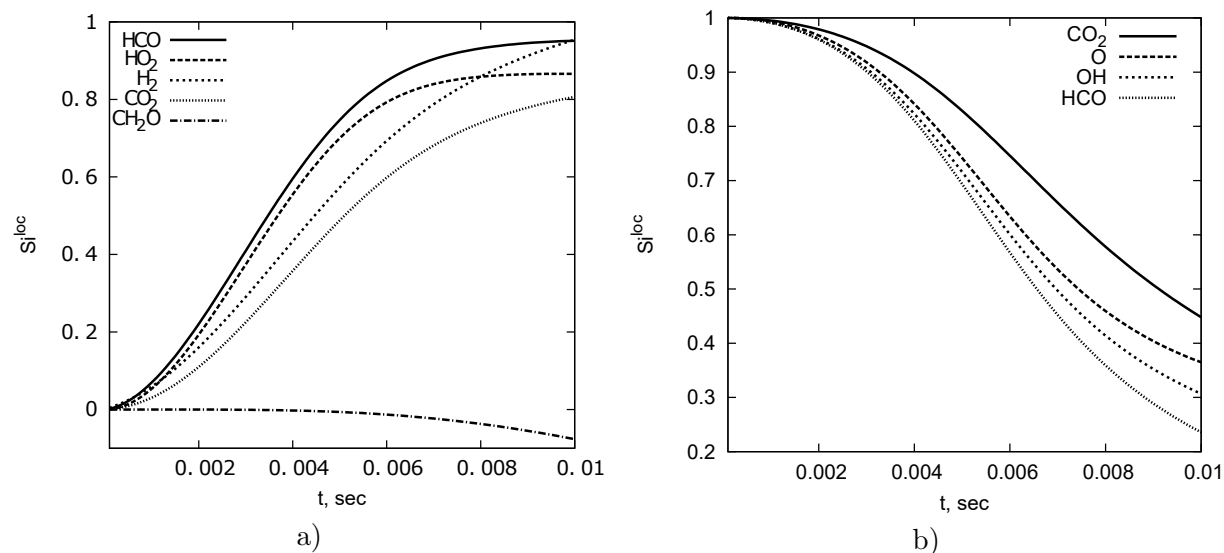
$$k_i = A_i \cdot e^{-E_i/RT}. \quad (2)$$

where  $E$  is the activation energy,  $A_i$  are kinetic parameters,  $R$  is the universal gas constant,  $T$  is temperature.

## 3. Procedure of the sensitivity analysis of the mathematical model functional

In order to carry out the sensitivity analysis, it is necessary to calculate the sensitivity matrix of the output parameters to the variation of the input parameters for certain time points of the reaction [15]. This brings about the problem of how to analyze the obtained sets of matrices. If it is necessary to elucidate the scheme describing the process over a broad temperature range, the sensitivity analysis should be performed at different temperatures, because the sensitivity

coefficients can be considerably different (fig. 1). Interpretation of the obtained results is not so easy. In [8], calculation of averaged values was proposed for better interpretation, because in complex models with several input and output parameters, the matrix of sensitivity coefficients can be too large.



**Figure 1.** Local sensitivity analysis of changes in the concentrations of substances to changes in the rate constants 2 (a) and 22 (b).

In order to eliminate the possible difficulties in analysis of the sensitivity coefficients and to enhance the quality of reduction, we propose here the following procedure of sensitivity analysis. It is proposed to analyze the sensitivity of the model functional to variation of the rate constants (or to the Arrhenius kinetic parameters) where the functional determines how close the values calculated using the existing reaction scheme are to those calculated by the scheme obtained by perturbation of its parameters at various time points and/or for various temperatures:

$$F_{obj} = \sum_{i=1}^I \sum_{j=1}^J \sum_{m=1}^M (x_{ijm}^{sh1} - x_{ijm}^{sh2})^2, \quad (3)$$

where  $x_{ijm}^{sh1}$  are the concentrations calculated in terms of the initial scheme;  $x_{ijm}^{sh2}$  are concentrations calculated upon variation (perturbation) of parameters of the scheme.

Sensitivity analysis of the model functional identifies the parameters that make the largest (or smallest) contribution to the modeling result [16]. The mathematical model can contain parameters the variation of which does not affect the qualitative or quantitative process description. The contribution of these parameters to the functional would be minor. Therefore, the steps that do not serve for modeling of the kinetic curves of species can be eliminated from consideration. The order of the reduced scheme is dictated by the range of conditions (temperature, pressure, reaction time) for which the yields of species are to be adequately described. The functional includes summation over the reaction substances, several temperatures, and several time points. This is the way to obtain a reduced scheme consistent with the detailed scheme for the specified range of conditions.

There are global and local methods for analyzing the dependence of the solution of a set of kinetic equations on the reaction rate constants [17]. The global sensitivity analysis, unlike the local one, elucidates the behavior of kinetic curves over the whole range of parameters, estimates quantitatively the effect of particular variables and groups of variables, and identifies

the significant and insignificant parameters of the model. For calculating the global sensitivity coefficients, we chose the method proposed by I. M. Sobol' [18].

The sensitivity analysis method proposed by I. M. Sobol' is a total method based on decomposition of dispersions. It is fit for studying non-linear and nonmonotonic functions and models [19]. The first order sensitivity index  $S_i = D_i/D$  characterizes the contribution of dispersion of individual parameter  $x_i$  to the total dispersion of the function  $F_{obj}$ . The higher the value of the index is, the stronger the influence of the  $x_i$  variable on the  $F_{obj}$  function value. The total consideration of the influence of  $x_i$  variable requires to use the total sensitivity indices  $S_i^{tot}$ . The total sensitivity indices allow to estimate the impact of a single parameter on the variance of the model outcome, as well as the impact of all other possible combinations of parameters. The calculation of  $S_i^{tot}$  can be based on the variance  $D_{-i}$  that results from the variation of all parameters, except of  $x_i$  :

$$S_i^{tot} = S_i + \sum_{j \neq i} S_{ij} + \dots = \frac{D - D_{-i}}{D}. \quad (4)$$

#### 4. The results of computational experiments

For the formaldehyde oxidation reaction, the scheme used in the Kintecus V 5.20 program was chosen [20]. A detailed schemes for the formaldehyde oxidation mechanism is a large system that includes 15 reacting species and 25 steps of the reactions. The steps and the rate constants at a temperature of 952K are shown in Table 1.

In the study of this reaction, the following types of analysis were carried out:

- 1) the global sensitivity analysis of changes in the concentrations of substances to changes in the rate constants;
- 2) the global sensitivity analysis of the functional model to changes in the rate constants. In the present paper we determined the influence of the rate constants of the steps on the change of calculated concentration of a substance using the total sensitivity indices [21]. High-order integrals intended to obtain the sensitivity indices were calculated by the Monte Carlo method in the integration nodes that were generated in n-dimensional unit cube. During the global analysis, the constant for each step was varied within the interval  $[k_{i,min}, k_{i,max}]$ , where  $k_i$  is the rate constant in Table 1,  $k_{i,min} = k_i - \frac{h}{2} \cdot k_i$  and  $k_{i,max} = k_i + \frac{h}{2} \cdot k_i$  are the lower and upper values of the rate constant for  $i$ -th step,  $h$  is the perturbation value. The perturbation step in the reduction was 0.05. A variety of rate constants ( $2^{11}$  sets) were generated within the specified interval and the effect of variation of the constants on the functional was evaluated in terms of variances. We assumed the rate constants to be independent of one another. The rate constants were assumed to be independent of each other. A quasi-Monte Carlo method was used to provide the uniform distribution of possible values of the rate constants. Points of the LP $\tau$  sequence proposed by I.M. Sobol served as quasi-random points. The CPU time required is two-three hours to perform the sensitivity analysis.

Table 2 summarizes the results of sensitivity analysis of the calculated concentrations to the variation of reaction rate constants. We chose not to present the values of sensitivity indices, but for clarity presented them as a table, where the steps are numbered in the order of significance for each species. For example, according to Table 2, at the expense of the main reagent reaction is formaldehyde the most affected by the variation of the rate constant  $k_2$  for the second step  $HO_2 + CH_2O \rightarrow H_2O_2 + HCO$ , then the rate constant  $k_{22}$  for the step  $CH_2O + O_2 \rightarrow HCO + O_2$  and so on. Only those steps were numbered for which sensitivity coefficient  $S_i^{tot}$  was more than  $10^{-6}$ . Correspondingly, if for all output parameters, the sensitivity to parameters of some step was below this value, this step was not included in Table 2.

One can see that variation of the constants of the steps of chain propagation cycle and the degenerate branching of the chain, namely, steps 2, 3, 10, 22, produced the least effect

**Table 1.** The detailed schemes for the formaldehyde oxidation mechanism and its parameters.

No.	Step	$k_i$
1	$HCO + O_2 \rightarrow HO_2 + CO$	$6.02 \cdot 10^{10}$
2	$HO_2 + CH_2O \rightarrow H_2O_2 + HCO$	$3.43 \cdot 10^{10}$
3	$H_2O_2 + M \rightarrow 2OH + M$	$4.01 \cdot 10^6$
4	$OH + CH_2O \rightarrow H_2O + HCO$	$9.64 \cdot 10^{13}$
5	$OH + H_2O_2 \rightarrow H_2O + HO_2$	$3.07 \cdot 10^{12}$
6	$H_2O_2 \rightarrow H_2O_2^-$	$1.05 \cdot 10^2$
7	$HO_2 \rightarrow HO_2^-$	$1.05 \cdot 10^1$
8	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$1.81 \cdot 10^{12}$
9	$OH + CO \rightarrow CO_2 + H$	$1.99 \cdot 10^{11}$
10	$HO_2 + CO \rightarrow CO_2 + OH$	$7.23 \cdot 10^8$
11	$H + CH_2O \rightarrow H_2 + HCO$	$1.63 \cdot 10^{12}$
12	$H + O_2 \rightarrow OH + O$	$3.32 \cdot 10^{10}$
13	$H + O_2 + M \rightarrow HO_2 + M$	$3.63 \cdot 10^{15}$
14	$HO_2 + M \rightarrow H + O_2 + M$	$2.83 \cdot 10^5$
15	$O + H_2 \rightarrow OH + H$	$1.82 \cdot 10^{11}$
17	$H + H_2O_2 \rightarrow HO_2 + H_2$	$7.83 \cdot 10^{11}$
18	$H + H_2O_2 \rightarrow H_2O + OH$	$3.55 \cdot 10^{12}$
19	$O + H_2O_2 \rightarrow OH + HO_2$	$6.02 \cdot 10^{10}$
20	$HCO \rightarrow H + CO$	$4.60 \cdot 10^{-12}$
21	$OH + H_2 \rightarrow H_2O + H$	$6.02 \cdot 10^{12}$
22	$CH_2O + O_2 \rightarrow HCO + HO_2$	$1.75 \cdot 10^4$
23	$H + HO_2 \rightarrow 2OH$	$3.01 \cdot 10^{12}$
24	$H + HO_2 \rightarrow H_2O + O$	$3.01 \cdot 10^{13}$
25	$H + HO_2 \rightarrow H_2 + O_2$	$2.71 \cdot 10^{13}$

**Table 2.** Significant steps with sensitivity rankings for each substances.

$k_i$	$HCO$	$O_2$	$HO_2$	$CO$	$CH_2O$	$H_2O$	$CO_2$	$H_2$
$k_1$	2	10	10	9	10	10	10	10
$k_2$	1	1	3	1	1	4	4	6
$k_3$	3	4	1	3	4	3	3	5
$k_4$	8	6	6	8	6	9	6	2
$k_6$	11		11			12		
$k_8$	6	7	4	5	8	6	7	9
$k_9$	7	5	5	7	5	8	5	1
$k_{10}$	5	3	8	11	3	1	1	3
$k_{11}$	10	9	9	6	9	7	9	7
$k_{12}$	9	8	7	4	7	5	8	
$k_{13}$	12	11	12	10	11	11		8
$k_{22}$	4	2	2	2	2	2	2	4

on the calculated concentrations. In general, the influence of only these steps determines the dynamics of the formaldehyde concentration. Only those steps were presented for which sensitivity coefficient  $S_{itot}$  was more than 10–3.

In addition to this analysis identifying the most and least influential steps of the process, also the analysis of the sensitivity of functional  $F_{obj}$  to the change of the rate constants of steps was carried out. Table 3 presents the sensitivity of functional  $F_{obj}$  to variation of the rate constants of steps. Functional  $F_{obj}$  characterizes closeness of the measured values to simulated values by scheme (Table 1). Values of rate constants of the steps changed over the same range as in previous analysis.

**Table 3.** The reduced scheme for formaldehyde oxidation reaction.

No.	Step	$S_i^{tot}$
22	$CH_2O + O_2 \rightarrow HCO + HO_2$	0.627
2	$HO_2 + CH_2O \rightarrow H_2O_2 + HCO$	0.588
10	$HO_2 + CO \rightarrow CO_2 + OH$	0.311
3	$H_2O_2 + M \rightarrow 2OH + M$	0.199
9	$OH + CO \rightarrow CO_2 + H$	0.028
4	$OH + CH_2O \rightarrow H_2O + HCO$	0.028
12	$H + O_2 \rightarrow OH + O$	0.025
8	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	0.020
1	$HCO + O_2 \rightarrow HO_2 + CO$	0.006
13	$H + O_2 + M \rightarrow HO_2 + M$	0.003
11	$H + CH_2O \rightarrow H_2 + HCO$	0.002

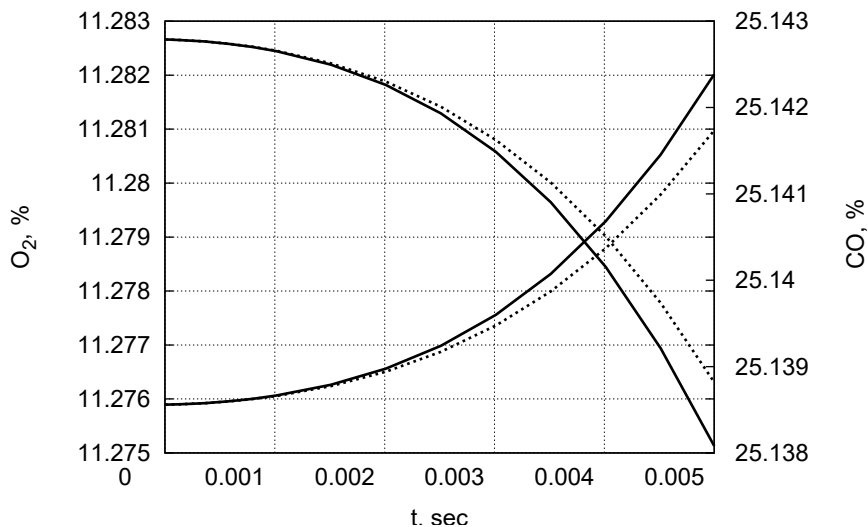
While investigating the sensitivity of the model functional coefficients to the variation of model parameters, we took into account the variation of the squared temperature difference at a specified time point and the concentrations for the following species:  $O_2$ ,  $HO_2$ ,  $CO$ ,  $CH_2O$ ,  $H_2O$ , and  $CO_2$ . The values found by numerical solution of system (1) at five time points with the following initial conditions:  $CH_2O$  concentration,  $1.124 \cdot 10^{-7} mol/cm^3$ ;  $O_2$  concentration,  $2.109 \cdot 10^{26} mol/cm^3$ ;  $CO$  concentration,  $4.699 \cdot 10^{-6} mol/cm^3$ ; temperature, 952 K were taken as the values. On the basis of the results of analysis, the steps were ranked in the order of significance. Then the least significant steps were successively excluded until the relative deviation between the values calculated in terms of the two schemes exceeded 2%. Table 3 shows the most significant steps of the process. It is seen that the value of functional  $F_{obj}$  is greatly affected by parameters of steps 2, 3, 10, 22.

The resulting (reduced) scheme consisting of 14 steps and describes the behaviors of all species in the same way as the detailed scheme (fig. 2). Thus, 14 steps can be excluded from the consideration without a substantial change in the kinetic modeling results.

### 5. Computational aspects of the problem solution

We indicate some computational aspects of the problem solution. The reduction results for the reaction scheme depend on them.

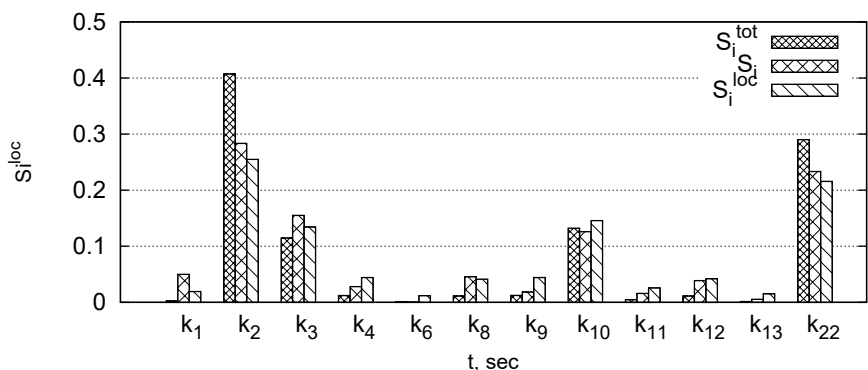
The global method allows us to analyze functions in which there are non-linear interactions between parameters. Taking into account the joint interaction of the parameters  $k_i$  and  $k_j$  plays an important role in the simulation, since the reaction scheme includes steps of the second order. Therefore, we calculated the total sensitivity coefficients, which include first and second order sensitivity coefficients:



**Figure 2.** The temporal profiles of basic substances concentrations (the solid line is the calculation for the detailed scheme, a dashed line is the calculation for the reduced scheme).

$$S_i^{tot} = S_i + \sum_{j \neq i} S_{ij}. \tag{5}$$

Figure 3 shows a graph of comparative analysis for local and global first-order sensitivity coefficients and total global sensitivity coefficients of the formaldehyde concentration to changes of some rate constants. We used different approaches to calculate the local and global sensitivity coefficients of the first order, nevertheless the results of the analysis showed a similar result. The difference between total global sensitivity coefficients and global sensitivity coefficients of the first order is explained by the fact that the cumulative change of two rate constants of the steps, namely, the variation of parameters 2, 11, 22 steps with other parameters, has a significant effect on the description of the process.



**Figure 3.** Comparative analysis for local and global first-order sensitivity coefficients and total global sensitivity coefficients of the formaldehyde concentration to changes of some rate constants.

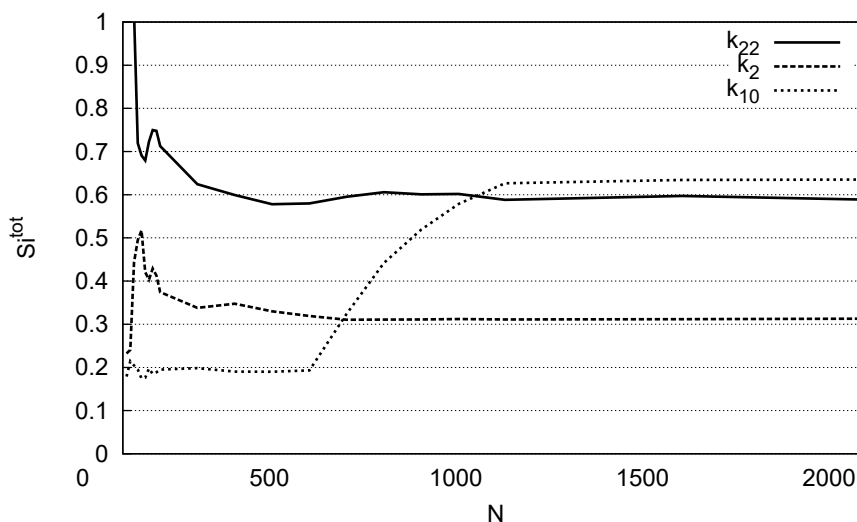
During the global analysis, the constant for each step was varied within the interval  $[k_{i,min}, k_{i,max}]$ , where  $k_i$  is the rate constant in Table 1,  $k_{i,min} = k_i - \frac{h}{2} \cdot k_i$  and  $k_{i,max} = k_i + \frac{h}{2} \cdot k_i$  are the lower and upper values of the rate constant for  $i$ -th step,  $h = 0.05$  is the perturbation

value. It should be noted that the values of the sensitivity coefficients do not strongly depend on the small value of  $h$  (Table 4).

**Table 4.** Total global sensitivity coefficients for different  $h$ .

No.	Step	$h = 0.02$	$h = 0.5$	$h = 0.1$
22	$CH_2O + O_2 \rightarrow HCO + HO_2$	0.627	0.656	0.666
2	$HO_2 + CH_2O \rightarrow H_2O_2 + HCO$	0.588	0.618	0.629
10	$HO_2 + CO \rightarrow CO_2 + OH$	0.311	0.311	0.309
3	$H_2O_2 + M \rightarrow 2OH + M$	0.199	0.200	0.198
9	$OH + CO \rightarrow CO_2 + H$	0.028	0.028	0.028
4	$OH + CH_2O \rightarrow H_2O + HCO$	0.028	0.027	0.027
12	$H + O_2 \rightarrow OH + O$	0.025	0.026	0.026
8	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	0.020	0.019	0.019
1	$HCO + O_2 \rightarrow HO_2 + CO$	0.006	0.006	0.006
13	$H + O_2 + M \rightarrow HO_2 + M$	0.003	0.003	0.003
11	$H + CH_2O \rightarrow H_2 + HCO$	0.002	0.002	0.002

The accuracy of calculating global sensitivity coefficients depends on the number of sets of constants generated within the interval  $[k_{i,min}, k_{i,max}]$ .  $2^{10}$  - the optimal number of points at which the values of the sensitivity coefficients are constant (fig. 4).



**Figure 4.** Dependence of total global sensitivity coefficients on the number of generated sets  $N$ .

Also, undoubtedly, the results of reduction depend on the criterion for choosing the steps. Values of global sensitivity coefficients are normalized and can take values between 0 and 1. The reduced reaction scheme includes only those steps for which the sensitivity coefficient is greater than a certain value. Thus, it is possible to determine the degree of simplification of the scheme and, accordingly, the accuracy of the description of the reaction by the reduced scheme. In this paper the steps were ranked according to the descending values of the functional. The criterion for reduction was as follows: the least significant steps were successively excluded



until the relative deviation between the values calculated in terms of the of detailed and reduced schemes exceeded 2%.

## 6. Conclusion

Thus, we developed a procedure for constructing reduced schemes of chemical reactions predicting the concentrations and the major yields of reactions to the desired accuracy and distinguished by moderate requirements to computing resources. The obtained data on the sensitivity of the functional may be useful for optimization of solution of the inverse chemical kinetics problem. Using this procedure, the kinetic scheme of formaldehyde oxidation reaction was investigated that includes 15 reacting species and 25 steps of the reactions. The analysis established the key steps of the formaldehyde oxidation reaction affecting the overall dynamics. The reduced scheme for formaldehyde oxidation scheme was established, that describes the same behavior of the principal reaction species under atmospheric pressure as the detailed. The paper presents computational aspects of the solution of the problems of chemical kinetics by the global sensitivity method using the example of the formaldehyde oxidation reaction.

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