

Prediction of State-to-State Dissociation Rate Coefficients Using Machine-Learning Algorithms

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Abstract—We study the possibility of using machine-learning algorithms to optimize the prediction of state-to-state (STS) dissociation rate coefficients in modeling nonequilibrium air flows. A rigorous but computationally complex theoretical model of reaction-rate coefficients, which considers the electronic and vibrational excitation of all reaction participants (products and reagents), is taken as a basis. Several algorithms are considered for predicting the STS dissociation rate coefficients of air components: k-nearest neighbors (k-NN) and decision tree (DT) regression, as well as neural networks; their accuracy and efficiency are analyzed. It is shown that the use of regression (k-NN and DT) algorithms is inappropriate for our problem, while neural-network algorithms have clear advantages over classical regression algorithms in terms of time and scalability. Validation of the neural-network approach is carried out by considering the example of solving the problem of vibrational-chemical relaxation behind a shock wave. A satisfactory agreement with the experiment and almost complete coincidence of the results with the solution obtained by theoretical methods without the use of machine learning are shown. The approach to data representation and processing proposed in this paper is easily scalable to more complex models taking into account the excitation of internal degrees of freedom. Thus, when taking into account the electronic excitation of a molecule, acceleration of about 1–2 orders is achieved without significant loss of accuracy. As a result, this study demonstrates that the use of neural-network methods makes it possible to predict state-specific reaction-rate coefficients with a high degree of accuracy without performing direct calculations using resource-intensive theoretical formulas directly in the working code. The approach scales as the complexity of the formulation increases (as is shown in the case of taking into account the electronic-vibrational excitation of the reagents), which allows us to reduce the time required to perform the calculations. At the same time, such a result is achieved through serious preliminary work and requires the development of large arrays of preliminary data. If we automate this process using a neural network, we can obtain a computationally efficient tool for systematic predictions of state-to-state reaction-rate coefficients.

Keywords: chemical reaction rate, state-to-state kinetics, dissociation, nonlinear regression, machine learning, neural network, optimization of numerical calculations

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1. INTRODUCTION

Simulations of high-temperature nonequilibrium gas flows are of great importance for aerospace research. Thus, for example, to design the thermal-protection systems of reentering vehicles, it is important to predict with a high accuracy the rates of chemical reactions of dissociation, recombination, and exchange that occur near its surface. The application of molecular dynamics, quantum mechanical, and quasi-classical trajectory (QCT) calculations [1–5] provides the most accurate data; however, these approaches cannot be directly integrated into computational fluid dynamic codes, since the direct calculation of state-to-state reaction rates depending on temperature and all possible vibrational states of reagents and products requires a lot of time and computational resources. Therefore, in practice, theoretical models of reaction-rate coefficients [6–9] are widely used. It is typical for modern models [8, 9] to

have a high accuracy and satisfactory agreement with QCT data, however, they contain resource-consuming computational parts, which significantly slow down calculations and limit the class of problems which can be solved by using these models. In this context, the problem of obtaining reaction-rate coefficients by using more rapid and efficient methods arises.

Methods of machine learning and neural networks are powerful tools to predict, generalize, and accelerate calculations of different types, which had earlier rather a theoretical character. The first attempts to use machine learning for solving state-to-state kinetics problems were performed in [10–14] to calculate vibrational relaxation rates and transport coefficients. In our study, machine-learning methods are used for approximate calculation and speed-up of the calculation of dissociation-rate coefficients in air with possible further scaling of the program modules obtained for predictions of the rates of physical-chemical processes to arbitrary reactions and temperatures.

2. THEORETICAL MODEL

Numerous studies are devoted to investigation of the rates of chemical reactions in the state-to-state approximation [1–5]. The majority of them consider only the states of a decaying or exchanging molecule without consideration of the states of other participants of the collision or reaction products. In Aliat's work [7], a theoretical model of chemical reactions considering the electronic-vibrational excitation of a reagent molecule is presented. Unfortunately, this model is not widely used because of misprints in the initially published text, which were found and corrected in [15]. In further studies, based on the model of [8], a generalized formula was obtained to calculate the chemical-reaction rate coefficients in the state-to-state approximation with the possibility of taking into account the vibrational and electronic excitation of any number of reagents and reaction products [9]; in addition, it was shown that the Marrone—Treanor and Aliat formulas are particular extreme cases of this generalized formula.

According to [9], the generalized formula for calculating the dissociation- and exchange-reaction rate coefficients $k_{V_r \rightarrow V_p}^{\text{ex,diss}}$ taking into account the vibrational and electronic excitation of all the reaction participants is expressed in the form of the product of the thermally equilibrium reaction-rate coefficient $k^{\text{eq}}(T)$ and the nonequilibrium factor $\mathcal{Z}(T, V_r, V_p)$:

$$k_{V_r \rightarrow V_p}^{\text{ex,diss}} = k^{\text{eq}}(T)\mathcal{Z}(T, V_r, V_p), \quad (1)$$

$$\mathcal{Z}(T, V_r, V_p) = B(T) \exp\left(-\frac{\Delta\varepsilon_{V_r \rightarrow V_p} \cdot \Theta(\Delta\varepsilon_{V_r \rightarrow V_p})}{k} \left(\frac{1}{T} + \frac{1}{U}\right)\right), \quad (2)$$

$$\Delta\varepsilon_{V_r \rightarrow V_p} = \varepsilon_a + \varepsilon_p - \varepsilon_r, \quad (3)$$

where k is the Boltzmann constant; V_r and V_p are the internal states of the reaction reagents and products (in the model, both the molecules and atoms in arbitrary excited states are considered); ε_r and ε_p are the corresponding energies; $\Theta(x)$ is the Heaviside function; ε_a is the reaction activation energy; T is temperature; U is the model parameter that has a dimension of temperature; the thermally equilibrium reaction rate coefficient $k^{\text{eq}}(T)$ is determined according to the Arrhenius equation [9]; and B is the normalizing factor:

$$B(T) = \left(\sum_{V_r^*, V_p^*} \left[\exp\left(-\frac{\Delta\varepsilon_{V_r^* \rightarrow V_p^*} \cdot \Theta(\Delta\varepsilon_{V_r^* \rightarrow V_p^*})}{k} \left(\frac{1}{T} + \frac{1}{U}\right)\right) \prod_{l=1}^{M_r} n_{V_{r,l}^*}^{\text{eq}} \right] \right)^{-1}, \quad (4)$$

M_r is the number of reagents, $n_{V_{r,l}^*}^{\text{eq}}$ is the equilibrium molar fraction of the corresponding state of the l th reagent described by the Boltzmann distribution with the temperature T .

As is seen from the presented formula, when calculating the normalizing factor, it is necessary to sum the exponents of energy and temperature over the entire set of energy states of reaction participants. If we consider only the vibrational excitation of a dissociating diatomic molecule, the number of summed exponents will be several tens; however, when considering polyatomic molecules as well as the vibrational and electronic excitation of all the reaction participants (reagents and products), it will be nec-

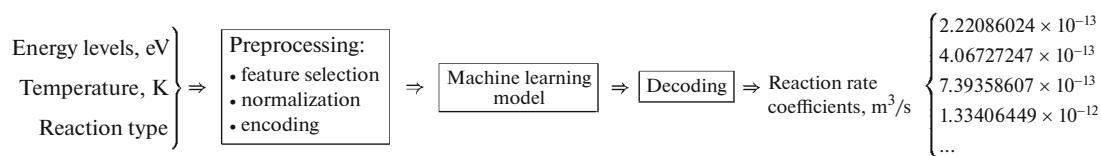


Fig. 1. Scheme of the ML model in the case of consideration of all vibrational levels of one reagent.

essary to consider the entire Cartesian product of electronic-vibrational states, which will give us, respectively, thousands and millions of terms. Therefore, acceleration of the calculation of the normalizing factor B (or the nonequilibrium factor \mathcal{Z}) with the help of machine learning (ML) methods is of great practical interest.

The first step in solving this problem with the aim of testing various ML algorithms is investigation of the simple extreme case, namely, the dissociation reaction taking into account the vibrational excitation of the decaying molecule alone. It is shown in [9] that formula (2) in such a case can be reduced to the well-known Marrone—Treanor formula [6]:

$$\mathcal{Z}_i(T, U) = \frac{Z^{\text{vibr}}(T)}{Z^{\text{vibr}}(-U)} \exp\left(\frac{\varepsilon_i}{k} \left(\frac{1}{T} + \frac{1}{U}\right)\right), \quad Z^{\text{vibr}}(T) = \sum_i \exp\left(-\frac{\varepsilon_i}{kT}\right), \quad (5)$$

where ε_i is the energy of the i th vibrational level, $Z^{\text{vibr}}(T)$ is the equilibrium partition function, and $Z^{\text{vibr}}(-U)$ is obtained by substituting the parameter $-U$ for temperature. It is obvious that this model is not too complicated from the computational point of view. However, it can be successfully used for testing ML algorithms, since it reflects the main peculiarities of the behavior of the state-to-state reaction-rate coefficients as functions of temperature.

3. IDEA OF USING ML MODELS IN THE PROBLEM OF CALCULATING COEFFICIENTS

When modeling complex mixtures with a large number of different molecules, the number of dissociation-rate coefficients for each calculation cell is hundreds; in the case of complex molecules, tens of thousands. For each temperature, it is necessary to calculate the complete set of coefficients, which requires summing exponents over all states. In the case of choosing another model of the energy spectrum (for example, using an anharmonic oscillator instead of a harmonic oscillator, changing the number of levels) or changing the values of model parameters, it is necessary to recalculate all the coefficients. Therefore, it seems to be useful to obtain the method for predicting the dissociation rate coefficients with sufficient accuracy without performing direct calculations for all possible values of temperature.

This problem can be reduced to the problem of neural networks and nonlinear regression. In the one-dimensional case, it is proposed to use as the input data the reaction temperature, reaction type ($\text{O}_2 + \text{O}$, $\text{O}_2 + \text{O}_2$, $\text{N}_2 + \text{N}$, $\text{N}_2 + \text{O}$, $\text{N}_2 + \text{N}_2$, $\text{NO} + \text{N}$, or $\text{NO} + \text{O}$), as well as the values of the zero vibrational level of the energy of molecules O_2 , NO , and N_2 (see Fig. 1). The use of the zero level of the vibrational energy ε_0 instead of all the energy values is preferable for training ML algorithms, since the pairwise correlation of energies ε_i may lead to the incorrect zero gradient in the process of neural-network training, thus, there is a chance to obtain the values of weights that do not reflect the actual dependence in the data.

When the electronic-vibrational states of molecules and the excitation of reaction products are taken into account, the data dimension increases according to the number of reaction participants for which we consider the electronic state.

To fit hyperparameters and enhance the reliability of the models of nonlinear regression from the sklearn library [16], the cross-validation method keeping the data out of the learning process was used. The recommended models are as follows:

—k-Nearest neighbors (k-NN) with the parameter of the number of neighbors $k = 3$ is an algorithm based on the assumption that for close objects in the feature space, there are similar output labels. Calculation and the model idea are quite simple, however, the time spent on prediction increases in accordance with the size of the trained data.

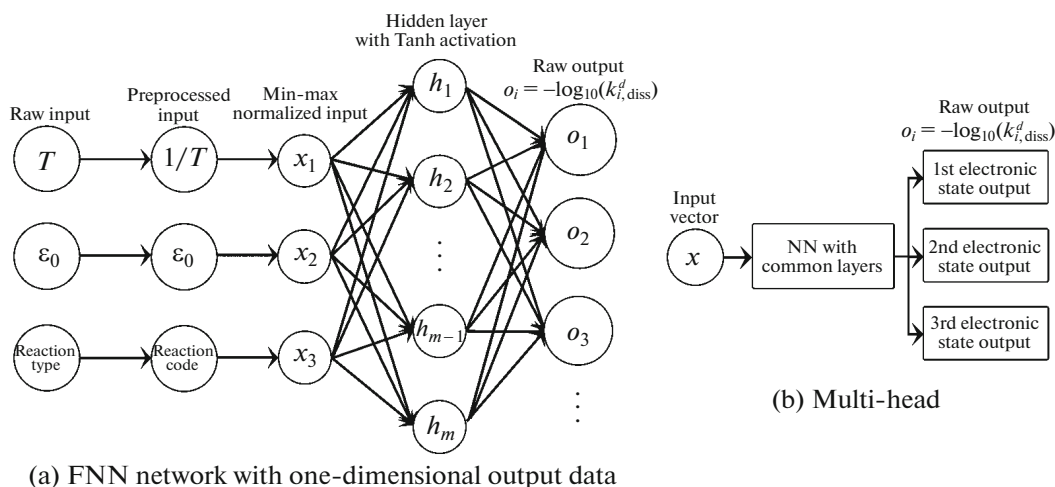


Fig. 2. Schemes of neural-network models considering data specifics.

—Decision tree (DT) with parameters $max_depth = 5$, $min_samples_leaf = 3$, $splitter = "random,"$ $max_features = "auto"$ is the algorithm representing a tree structure and does not require preliminary data normalization.

When applying the neural-network approach, the PyTorch library [17] was used; with the help of this library, a single-layer architecture Feedforward Neural Network (FNN) was realized; it is shown in Fig. 2a with 100 neurons in the hidden layer. As was noted above, in the case of consideration of electronic-vibrational excitation, the dimension of the investigated data increases: there is a unique value of energy for each electronic and each vibrational state of the chosen molecule. In such a case, it is possible to flatten the data (the Flatten transformation) or use the multi-head approach [18], which conserves the ideas of the one-dimensional case, however, uses in the last layer several outputs corresponding to the electronic states of the molecule (see Fig. 2b).

4. DATA ACQUISITION AND CHOICE OF METRICS

To generate the data set for training, a script was written in the Python 3.9, which calculates the set of state-to-state dissociation-rate coefficients depending on the set parameters: gas temperature, reaction type in terms of the set of reagents involved, and the spectrum of the vibrational energy for O_2 , NO , and N_2 molecules. The data were obtained in accordance with the exact theoretical model (1)–(2). At this stage, the script considers the excitation of one of the participants of the reaction, however, our approach is scalable for use in other mixtures or for corresponding data (energies of the vibrational levels, dissociation energies, etc.). Temperatures were considered within an interval from 1000 to 10000 K (the right boundary can be increased, for example, up to 15000 K without loss of model accuracy); in total, $100^{(n-1)}$ vectors were obtained with a subsequent division of this set into training and test sets, where n is the number of parameters which depends on the complexity of the theoretical model (for example, in the case of consideration of vibrational excitation alone, $n = 3$).

Data generation for considering the electronic excitation of molecules was performed in accordance with the anharmonic oscillator model and spectroscopic data for the electronic terms from [19].

Usually, the data preparation process for the model requires preliminary processing (except for DT). In our case, this is the min-max scaling of the input vectors and finding the logarithms of the target vectors. The latter is related to the fact that the physical values of the dissociation-rate coefficients vary within the interval from 10^{-70} to 10^{-14} m^3/s . The operation of ML models with such small values can be subjected to the problem of incorrect fitting of weights by the algorithm, which leads to high error values. The reaction type required special preliminary processing: since it is a categorical rather than numerical feature, each reaction type in air was represented in the form of an embedding vector [20] (here, representation through 0 and 1 according to the one-hot encoding [21] principle can also be suitable).

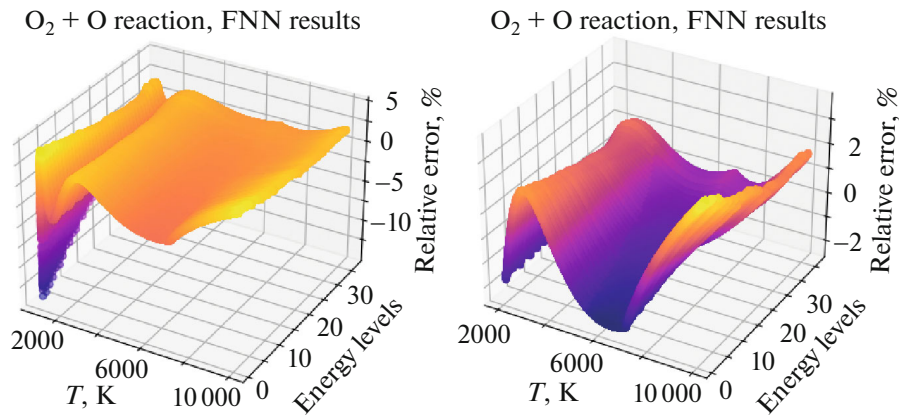


Fig. 3. Relative error of FNN predictions with (on the left) and without (on the right) taking into account temperatures lower than 2000 K in the case of vibrational excitation.

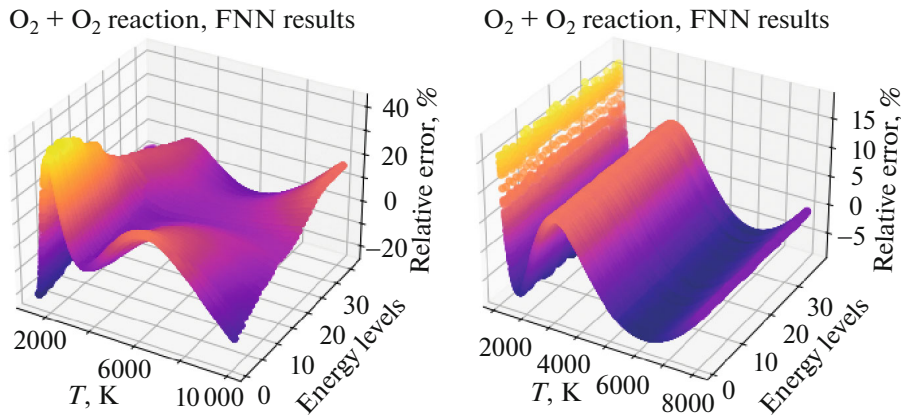


Fig. 4. Relative error of FNN predictions for the electronic state 1 (on the left) and electronic state 2 (on the right) for the case of electronic-vibrational excitation.

Working with values of small and rapidly changing orders, it is reasonable to consider the percent metrics to estimate the approximation quality; therefore, the mean absolute percent error was chosen:

$$\text{MAPE} = \frac{100\%}{n} \sum_{i=1}^n \left| \frac{y_i - \tilde{y}_i}{y_i} \right|, \quad (6)$$

where y_i is the theoretically calculated value and \tilde{y}_i is the value predicted by the model.

5. ESTIMATION OF ERROR AND TIME CONSUMPTION OF PREDICTION

Figure 3 shows the graph of the relative error of the values predicted by the FNN model. On the whole, it is possible to note that at temperatures higher than 2000 K, the built model demonstrates satisfactory agreement with the theoretical data. The results are similar in the case of taking into account electronic excitation (see Fig. 4). The increase in the error at low temperature values and at lower vibrational levels is associated with a physically abrupt change in the order of magnitude of the reaction-rate coefficients; this problem was considered in detail in [9]. To reduce the error at low temperatures (lower than 2000 K), it is possible to train an additional regression model. Nevertheless, when solving the majority of applied problems, the built model should provide a satisfactory accuracy, since an error of 10–15% in the vanishingly small reaction-rate coefficients at $T < 2000$ K does not influence the macroparameters of the non-equilibrium flow.

Table 1. Comparison of the mean test efficiency of calculating the coefficients in the case of the vibrational excitation of one molecule

Model	Time, ms	Acceleration, times	$\log_{10}(k_{\text{diss}})$ MAPE, %	k_{diss} MAPE, %
Theoretical	0.184	—	—	—
k-NN	0.349	0.53	0.001	0.015
DT	0.057	3.20	1.259	20.487
FNN	0.070	2.63	0.002	4.453

Table 2. Comparison of the mean test efficiency of calculating the coefficients in the case of the electronic-vibrational excitation of one molecule

Model	Time, ms	Acceleration, times	$\log_{10}(k_{\text{diss}})$ MAPE, %	k_{diss} MAPE, %
Theoretical	1.155	—	—	—
k-NN (Flatten)	0.346	3.33	0.001	0.093
DT (Flatten)	0.060	19.16	2.676	47.562
FNN (Flatten)	0.072	16.04	0.041	11.831
FNN (Multi-head)	0.130	8.88	0.016	6.893

Tables 1 and 2 present estimates of the accuracy and computational efficiency of the models: the mean general-system execution time (using a machine with x64 CPU IntelCore i7-9750H processor in the single-stream mode) of the block of code in Python 3.9 to obtain one desired vector. It is seen that k-NN algorithm and the FNN model give a good accuracy of prediction of the coefficients. It would be possible to solve the problem of the high DT algorithm error by ensembling basic models (random forest, gradient boosting [16]); however, this is not reasonable, since such an algorithm would significantly increase the computation time. When applying the k-NN regression, the computation time increases depending on the amount of data generated for training; therefore, if our aim is to speed-up the calculation, it is better to use FNN in this problem, which is confirmed by the results presented in Table 1. On the whole, we can come to the conclusion that for a simple model of calculation of the dissociation-rate coefficients (5), when we consider only the vibrational excitation of one participant of the reaction, the use of ML algorithms does not give a significant increase in the computational speed (Table 1) and is not recommended.

When considering the electronic excitation of the dissociating molecule (Table 2), the achieved speed-up is 1–2 orders of magnitude without significant losses of accuracy, which is evidence that it is reasonable to use ML algorithms when solving two- and three-dimensional problems of nonequilibrium gas dynamics. As was noted above, in the Flatten approach to data processing, one vector is predicted, which consists of the “flattened” matrix in which, at the intersection of the i th row and j th column, there is the dissociation-rate coefficient of the corresponding vibrational and electronic state of the molecule. In such an approach, the continuity of the predicted vector is lost, therefore, the error appears to be larger in comparison with that in the multi-head approach, where in the last layer, for each electronic state, there is a separate output from the FNN. Therefore, for the coefficient-prediction problem with consideration of the electronic excitation of reagents, it is recommended to use the multi-head approach.

It should be noted that the neural-network approach to data representation and processing described in this work is easily scalable to both the case of the electronic-vibrational excitation of all the participants of the reaction and the case of mixtures of polyatomic molecules, when the number of the reaction-rate coefficients required for each calculation cell is tens of thousands. The use of the neural-network approach when modeling nonequilibrium flows of such mixtures seems to be especially promising.

6. VALIDATION IN SIMULATIONS

The chemical-reaction rate coefficients are of interest, for simulations of gas mixture flows in the state-to-state kinetics approximation, when the necessity arises to solve systems of equations for macroparameters. For validation of the proposed approach, let us consider the flow behind a shock-wave in the state-to-state approximation [22].

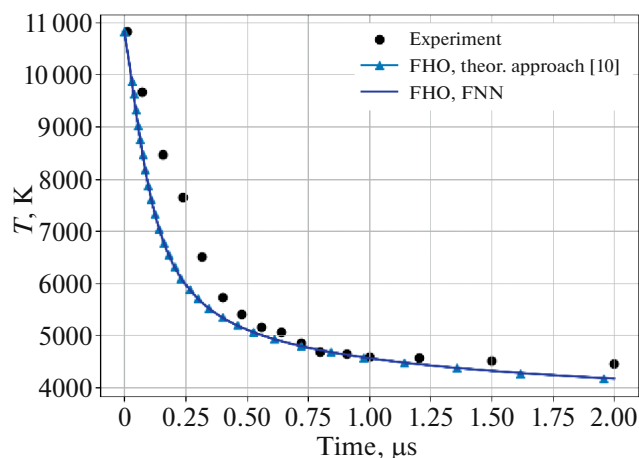


Fig. 5. Temperature profile behind the shock-wave front. O_2/O , $p_\infty = 0.8$ Torr, $M_\infty = 13.46$, $T_\infty = 299$ K.

The coefficients obtained with the help of the neural-network approach were integrated into the code for modeling the relaxation zone behind the shock wave in the O_2/O and N_2/N mixtures. Figure 5 shows the temperature profile of the gas behind the shock-wave front in the O_2/O mixture under the conditions of the experiment [23, 24]. The conditions in the free stream are as follows: $p_\infty = 0.8$ Torr, $M_\infty = 13.46$, $T_\infty = 299$ K. The vibrational-relaxation rate coefficients were calculated based on the theory of a forced harmonic oscillator [25]; the theoretical dissociation-rate coefficients were calculated according to the model [9]. The results obtained with the help of the neural-network approach nearly coincide with the theoretical results [9] (MAPE is 0.28%). It should also be noted that there is a satisfactory agreement of temperature with the experimental data.

7. CONCLUSIONS

As a result of this study, it is established that the use of machine-learning methods allow values of state-to-state chemical-reaction rate coefficients with a high accuracy to be obtained without performing direct calculations using labor-intensive theoretical formulas in the working code. Such an approach is scalable as the complexity of problem setting increases (as is shown in the case of taking into account the electronic-vibrational excitation of reagents), which makes it possible to significantly reduce the calculation time. At the same time, such a result is achieved by performing serious preliminary work and requires the development of large arrays of data describing all the variants of using the formulas (instead of one universal model, we need to create tens of new models). If this process is automated with the help of neural networks, it is possible to obtain a tool with a high calculation efficiency for performing systematic calculation of a similar type and preliminary estimations for the results of modeling flows in the state-to-state approximation.

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CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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