===== **MECHANICS** =====

# Neural-Network-Based Approach to the Description of Vibrational Kinetics of Carbon Dioxide

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**Abstract**—The nonequilibrium vibrational kinetics of carbon dioxide is modeled taking into account complex mechanisms of relaxation and energy exchanges between modes. The possibilities of using machine-learning methods to enhance the performance of the numerical simulation of nonequilibrium carbon-dioxide flows are studied. Various strategies for increasing the efficiency of the hybrid four-temperature model of $CO_2$ kinetics are considered. The neural-network-based approach proposed by us to calculate the rate of vibrational relaxation in each mode turns out to be the most promising. For the problem of spatially homogeneous relaxation, the error and computational costs of the developed algorithm are estimated, and its high accuracy and efficiency are demonstrated. For the first time, the carbon-dioxide flow behind a planar shock wave is simulated in a complete state-to-state approximation. The results obtained are compared with those in the hybrid four-temperature approach, and the equivalence of the approaches is shown. Based on this, the developed multi-temperature approximations may be recommended as the main tool for solving problems of nonequilibrium kinetics and gas dynamics. The hybrid four-temperature approach that uses a neural network for calculating relaxation terms reduces the numerical-simulation time by more than an order of magnitude while maintaining its accuracy. This technique can be recommended for solving complex multidimensional problems of nonequilibrium gas dynamics, including state-to-state chemical reactions.

**Keywords:** vibrational relaxation rate, state-to-state and multi-temperature kinetics, carbon dioxide, neural networks, machine learning

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## 1. INTRODUCTION

The study of the nonequilibrium kinetics of carbon dioxide is necessary for modeling the entry of descent vehicles into the atmospheres of Mars and Venus, for developing methods for reducing the concentration of products of human activity in Earth's atmosphere, in low-temperature plasma chemistry and laser technologies. A feature of the $CO_2$ molecule is that it has three vibrational modes (symmetric, bending, antisymmetric), which gives rise to several thousand bound vibrational states and leads to complex mechanisms of vibrational energy exchanges. Detailed state-to-state modeling, based on solving stiff differential equations for each state, is extremely demanding on computing resources. Consequently, there is a need to develop reduced models and efficient numerical methods.

To reduce computational costs in modeling nonequilibrium $CO_2$ flows, several state-of-the-art multi-temperature models have been developed that take into account energy exchange between modes [1, 2]. The main problem in using multi-temperature models lies in correct simulation of the rate of vibrational relaxation with consideration for various energy-exchange mechanisms. In the hybrid four-temperature model developed in [2], it was proposed to calculate the relaxation terms using averaged state-to-state rates of processes; due to this, the model retains its accuracy, but loses computational efficiency.

Along with conventional numerical methods, an approach has become popular in recent years, which consists in training neural networks to solve systems of differential equations [3, 4]. In such methods, neural networks are trained on the basis of a number of numerical solutions to a system of differential equations and enable the efficient calculation of system solutions for various sets of input-parameter conditions with a high degree of reliability. Although this approach is inapplicable in solving the problem of state-to-

state kinetics due to the high dimensionality of the system, its use for multi-temperature models seems to be promising.

In addition to the explicit use of neural networks for solving systems of differential equations, machine-learning methods can be applied to find local flow parameters or to approximate various characteristics. For example, neural networks have been used to find transport coefficients [5, 6]. In [7, 8], the application of a number of machine-learning methods in state-to-state modeling of the rate of vibrational relaxation in mixtures of air components was considered, but the results obtained cannot be used in multi-temperature approaches. Moreover, machine-learning methods have not been used before for modeling the kinetics of carbon dioxide. The only attempt made in [9] was related to the spectral clustering of energy levels.

The purpose of this work is to optimize calculation of the vibrational-relaxation rate in hybrid multi-temperature models based on machine-learning methods, to evaluate the accuracy and efficiency of neural-network approaches in solving problems of nonequilibrium gas dynamics, and to numerically simulate the problems of spatially uniform relaxation and the nonequilibrium flow of carbon dioxide behind a planar shock wave.

## 2. THEORETICAL MODEL

The use of a complete state-to-state model [10, 11] in studying the kinetics of $CO_2$ encounters significant difficulties due to the need to numerically solve a large number of differential equations for the populations of vibrational levels. Therefore, multi-temperature approaches are often used in practice, based on the fact that vibrational-energy-exchange rates can differ by several orders of magnitude; due to this, quasistationary vibrational distributions in different vibrational modes are established. To model the kinetics of carbon dioxide, multi-temperature approaches [2, 12] with vibrational-relaxation rates described by approximate Landau−Teller formulas are most often used. The limitations of these approaches are discussed in [1, 2, 11]. In particular, it was shown in [1] that the Landau−Teller model is only suitable for small deviations from equilibrium, while in [11] it was concluded that taking into account different temperatures in the symmetric and deformation modes provides the best agreement with the results of complete state-to-state simulation. In this paper, a four-temperature model is considered.

The four-temperature model is based on the assumption that intramode $VV_m$ ($m = 1, 2, 3$) exchanges of vibrational energy are fast processes, while all intermode $VV_{m-k}$ exchanges and $VT_m$ transitions of vibrational energy into translational energy are slow [2]. Under this condition, the set of macroparameters for a closed description of the nonequilibrium flow includes the density $\rho$ and the velocity $\mathbf{v}$ of the gas, the total specific energy $U$, and the temperatures of all vibrational modes $T_1$, $T_2$, and $T_3$. In this approach, the populations of the vibrational levels are given by the quasistationary distributions of Treanor (for an anharmonic oscillator) or Boltzmann (for a harmonic oscillator). The Treanor distribution in $CO_2$ has the form [11]

$$n_{i_1,i_2,i_3} = \frac{n s_{i_1,i_2,i_3}}{Z^{\mathrm{vibr}}(T,T_1,T_2,T_3)} \exp\left(-\frac{\varepsilon_{i_1,i_2,i_3} - (i_1\varepsilon_{1,0,0} + i_2\varepsilon_{0,1,0}, i_3\varepsilon_{0,0,1})}{k_\mathrm{B}T} - \frac{i_1\varepsilon_{1,0,0}}{k_\mathrm{B}T_1} - \frac{i_2\varepsilon_{0,1,0}}{k_\mathrm{B}T_2} - \frac{i_3\varepsilon_{0,0,1}}{k_\mathrm{B}T_3}\right), \qquad (1)$$

where $n$ is the numerical density of the gas; $s_{i_1,i_2,i_3} = i_2 + 1$ is the vibrational statistical weight; $\varepsilon_{i_1,i_2,i_3}$ is the vibrational energy of the level $(i_1, i_2, i_3)$; $k_\mathrm{B}$ is the Boltzmann constant; and $Z^{\mathrm{vibr}}$ is the vibrational partition function. Under such a description of the system, the total specific energy is a function of the gas temperature and all vibrational temperatures. For a harmonic oscillator, the first terms under the exponent are equal to zero, and distribution (1) transforms into the Boltzmann distribution.

The system of equations for an inviscid gas contains equations for the conservation of mass, momentum, and total energy, supplemented by relaxation equations for the specific numbers of vibrational quanta in various modes $W_m$:

$$\frac{d\rho}{dt} + \rho\nabla \cdot \mathbf{v} = 0, \qquad (2)$$

$$\rho\frac{d\mathbf{v}}{dt} + \nabla p = 0, \qquad (3)$$

$$\rho\frac{dU}{dt} + p\nabla \cdot \mathbf{v} = 0, \qquad (4)$$

$$\rho\frac{dW_m}{dt} = R_m, \quad m = 1, 2, 3, \qquad (5)$$

where $p$ is the pressure and $R_m$ is the relaxation rate in the $m$th mode. The specific numbers of vibrational quanta $W_m$ in the $m$th mode are introduced by the formulas:

$$\rho W_m(T, T_1, T_2, T_3) = \sum_{i_1, i_2, i_3} i_m n_{i_1, i_2, i_3}, \qquad m = 1, 2, 3, \tag{6}$$

$i_m$ is the vibrational quantum number corresponding to the $m$th mode. The introduction of the total specific energy $U$ and the specific number of vibrational quanta $W_m$ in each vibration mode as macroscopic variables is equivalent to the introduction of the gas temperature $T$ and three vibrational temperatures of the symmetric, bending, and asymmetric modes of $CO_2$ molecules ($T_1$, $T_2$, $T_3$).

An important feature of the presented multi-temperature (4T) model is that the approximate Landau–Teller formulas are not used for calculating the relaxation terms $R_m$. In this model, they are found by averaging the state-to-state relaxation terms $R_{i_1, i_2, i_3}^{\mathrm{vibr}}$ [2]:

$$R_m = \sum_{i_1, i_2, i_3} i_m R_{i_1, i_2, i_3}^{\mathrm{vibr}}, \qquad m = 1, 2, 3. \tag{7}$$

For example, for VT exchange in the bending mode, the relaxation term has the form

$$R_{i_1, i_2, i_3}^{\mathrm{VT}_2} = n_{i_1, i_2 - 1, i_3} k_{i_2 - 1 \to i_2} + n_{i_1, i_2 + 1, i_3} k_{i_2 + 1 \to i_2} - n_{i_1, i_2, i_3} (k_{i_2 \to i_2 - 1} + k_{i_2 \to i_2 + 1}), \tag{8}$$

where $k_{i \to i'}$ are the rate coefficients of the corresponding transitions.

An advantage of such a hybrid approach is good agreement between the results of modeling nonequilibrium carbon-dioxide flows with those of a complete state-to-state calculation, along with a significant reduction in the number of differential equations: from several thousand to six. Nevertheless, the disadvantage of the hybrid approach is the high computational cost in calculating the relaxation terms, which is comparable to using the complete state-to-state approach.

To solve system (2)−(5), the rate coefficients of energy transitions in each of the vibrational states should be calculated. In some situations, experimental data can be used, but these data are limited to lower states and low temperatures (less than 2000 K) and do not describe all types of energy exchanges. In the absence of experimental data, approximate theoretical models have to be used. In this study, the energy-transition-rate coefficients are found from the formulas of Schwartz, Slawsky, and Herzfeld [13] generalized to the case of an anharmonic oscillator (the SSH model). To increase the efficiency of calculating the coefficients, the data structure described in the previous work [14] is used.

## 3. NEURAL-NETWORK-BASED APPROACHES TO THE OPTIMIZATION OF CALCULATIONS

We now consider some approaches to optimizing the above problem. The first chosen strategy involved the application of machine-learning methods to the direct solution of a system of differential equations. The classic way to optimize the solution of a dynamic system is to replace the solver with a neural network trained on a number of solutions. The efficiency of such an approach for systems of ordinary differential equations and systems of partial differential equations has been shown in [4]. However, in the case of rigid systems, too large a sample of values and training for a large number of epochs are needed, which leads to the problem of overfitting, i.e., situations when the neural network yields accurate predictions on elements from the test sample and significant deviations on the remaining values.

An alternative approach to speeding up kinetics simulations is to use artificial-intelligence algorithms to quickly perform computationally complex steps of a numerical method, such as calculating relaxation terms. It was shown in [8] that machine-learning methods are much less sensitive to an increase in the dimension of a system of differential equations than standard numerical algorithms. Analysis of the possibilities of machine-learning methods to predict the values of relaxation terms in the system of equations for the complete state-to-state kinetics of carbon dioxide showed that such an approach would not give a positive effect, since the number of calculated relaxation terms is asymptotically equal to the number of actions performed when they are explicitly calculated. Thus, a more realistic approach is to improve the algorithm for modeling the kinetics of carbon dioxide in the hybrid 4-temperature approximation by approximating the values of the relaxation terms.

The most common approaches for approximating functions using machine-learning algorithms are: regression analysis; methods based on the k nearest neighbors (k-NN) algorithm; and the neural-network approach. Finding a regression model that makes it possible to achieve a high accuracy of approximation for the relaxation terms of each of the modes is an extremely difficult task due to strong nonlinearity of the
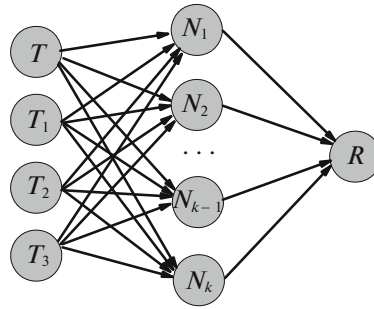
**Fig. 1.** Neural-network topology graph.

temperature dependence of these values. Simple linear and nonlinear methods are applicable in a narrow temperature range (the interval does not exceed 50 K). Thousands of simple regression models for each energy level would need to be trained to cover the entire 4D temperature range and using this approach would not be more efficient than direct calculation.

Study [7] considered the applicability of approximations based on the k-NN and gradient boosting methods for calculating relaxation terms in modeling the kinetics of a binary mixture in the state-to-state approximation. Comparison showed that the k-NN-based approach proved to be the most effective in calculations based on coefficients of the energy-transition rates according to the computationally expensive model of a forced harmonic oscillator (FHO) [1, 15]. However, if the computationally simple SSH theory is used, explicit calculation is much more efficient than the considered machine-learning methods. Since this work uses the SSH model and approximations based on its regression, it was concluded that it is inappropriate to use the k-NN methods and gradient boosting.

We now consider an alternative strategy based on the neural-network approach. According to the Tsybenko theorem (Universal approximation theorem), a feedforward artificial neural network with one hidden layer can approximate any continuous function of many variables with any accuracy. The conditions for such an approximation are: a sufficient number of hidden-layer neurons, a good choice of weights between input neurons and hidden-layer neurons, weights between connections from hidden-layer neurons and an output neuron, and biases for input-layer neurons.

For numerical experiments, three neural networks were used with the following topology (Fig. 1):

(i) a single-layer network topology model with direct access was used due to the fact that the neural network is used as a regression model;

(ii) the size of the input layer corresponds to the number of input variables: four temperature values;

(iii) the size of the output layer corresponds to the number of desired values: one relaxation term for the corresponding vibrational mode;

(iv) the hidden layer consists of 100 neurons for the first and second modes and 200 for the third mode; and

(v) a hyperbolic tangent was used as the activation function.

To train neural networks, samples were generated consisting of approximately $5\,000\,000$ temperature vectors $(T, T_1, T_2, T_3)$ and their corresponding relaxation terms $(R_1(T, T_1, T_2, T_3), R_2(T, T_1, T_2, T_3), R_3(T, T_1, T_2, T_3))$. These vectors were chosen taking into account the distribution density of temperature values arising at the steps of modeling spatially homogeneous carbon dioxide relaxation in the 4-temperature approximation. The neural network was trained in *Python* using the *scilearn* library. The creation of the training and testing set, which is a computationally extremely time-consuming operation, takes about two weeks. Training of each neural network requires about 4 hours. However, neural networks are trained only once, and the training results are used to solve various problems.

A trained neural network makes it possible to obtain predicted values of relaxation terms close to accurate ones for temperatures far from the boundaries of the interval on which they were trained. At temperatures from 2200 to 8000 K, the difference between the predicted and explicitly calculated values of the relaxation terms does not exceed 1%. If the area is extended while maintaining such accuracy, the neural network needs to be retrained. Therefore, if the range of temperature variation is assumed to be wider in the hydrodynamic problem under consideration, it is necessary to build several neural networks corresponding to different subsets of the complete temperature range. However, the use of several neural networks does not lead to a noticeable complication of the problem and a decrease in the calculation speed.
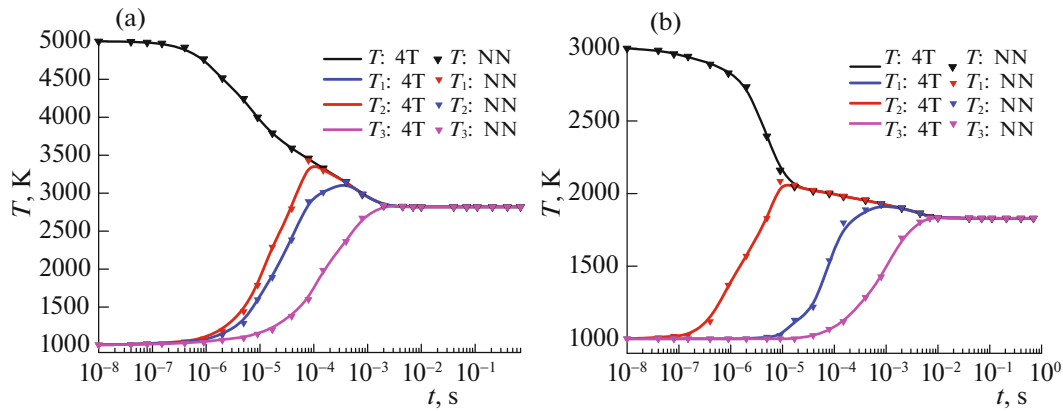
**Fig. 2.** Temperature distribution in the hybrid multi-temperature approximation for the explicit (4T) and neural network (NN) methods for calculating relaxation terms under conditions $TC1$ (a) and $TC2$ (b).

The obtained neural networks were integrated into the code for modeling the spatially homogeneous relaxation of carbon dioxide in the hybrid 4-temperature approximation. To this end, based on the obtained weight coefficients, neural networks were implemented in C++. After testing the neural networks on test samples, spatially homogeneous carbon dioxide was modeled in the four-temperature approximation based on the predicted values of the relaxation terms. The data were divided into training and test sets in the proportion of 2 : 3. The relative error of the solution based on the approximation of relaxation terms does not exceed 4%.

## 4. RESULTS AND DISCUSSION

In the numerical simulation of spatially homogeneous carbon dioxide in the state-to-state and four-temperature approximations, a code based on the AT-EBDF-4 numerical scheme [10] was used. Several test cases were considered with various initial conditions typical of different types of flows. In all cases, the initial pressure was assumed to be 100 Pa. The initial values of the temperature and vibrational temperatures of each mode were:

$TC1$: $T = 5000$ K, $T_1 = T_2 = T_3 = 1000$ K;

$TC2$: $T = 3000$ K, $T_1 = T_2 = T_3 = 1000$ K;

$TC3$: $T = 490$ K, $T_1 = T_2 = 490$ K, $T_3 = 2000$ K;

$TC4$: $T = 400$ K, $T_1 = T_2 = 500$ K, $T_3 = 1070$ K;

$TC5$: $T = 3000$ K, $T_1 = 300$ K, $T_2 = 700$ K, $T_3 = 1200$ K.

Figure 2 shows the time dependences of the temperatures $T$, $T_1$, $T_2$, and $T_3$ for the cases $TC1$ and $TC2$ that correspond to the conditions in shock waves. The temperatures are calculated in the hybrid 4T approximation with explicit calculation of the relaxation terms and using the neural-network approach. The solutions obtained using neural networks are in good agreement with the accurate 4T solutions: the maximum error for all temperatures does not exceed 1.5%, which is a very good result. In both cases, the fastest relaxation is observed in the bending mode, while the antisymmetric mode reaches equilibrium much more slowly than the other modes. If the initial temperature increases, the relaxation rates of the first and second modes become close, and the time to reach complete equilibrium decreases.

We now consider two examples with initial conditions typical for discharges (Fig. 3). The case $TC_3$ corresponds to capillary discharges in laser mixtures; in this case, the antisymmetric mode is significantly excited, while the symmetric and deformation modes are in equilibrium with the translational-rotational modes. The temperature distribution calculated in the 4T approximation for this case shows that in the process of relaxation the balance between $T$, $T_1$ and $T_2$ is not violated, and relaxation occurs through the antisymmetric mode ($VT_3$ and intermode $VV_{2-3}$, $VV_{1-2-3}$ exchanges). Test case $TC4$ corresponds to glow-discharge conditions with a slight excitation of the symmetric and bending modes and significant excitation of the antisymmetric mode. In this case, the relaxation of the first and second modes occurs rapidly, in less than a microsecond, while the relaxation of the antisymmetric mode lasts for several seconds. There
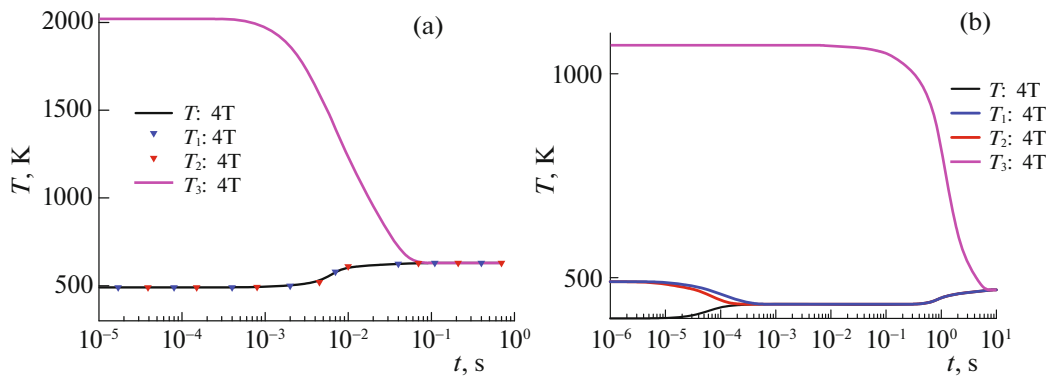
**Fig. 3.** Temperature distribution in the hybrid multi-temperature approximation for the explicit method for calculating relaxation terms under conditions $TC3$ (a) and $TC4$ (b).
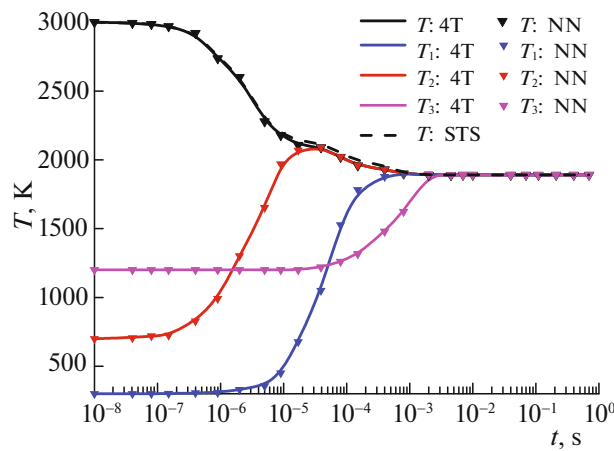


**Fig. 4.** Temperature distribution in the state-to-state (STS), hybrid multi-temperature approximation for explicit (4T) and neural network (NN) methods for calculating relaxation terms under conditions $TC5$.

is a slight difference in the rate of $T_1$ and $T_2$ relaxation; the temperature of the bending mode comes close to $T$ somewhat earlier.

Test case $TC5$ with significantly different initial temperatures for all modes was chosen to demonstrate the performance of the proposed approaches. It has no explicit physical analogue, but can be used as a test for the correctness of the code. The use of all approaches (complete state-to-state, 4T with different ways of calculating relaxation terms) yields similar results (Fig. 4), but the neural-network approach is much more efficient from the computational perspective.

The effectiveness of the different approaches is compared in Table 1. If the neural-network approach is used, the speed of calculating relaxation terms in the multi-temperature approximation increases by a factor of more than 17. The general solution of the system is found an order of magnitude faster. It should be noted that the maximum relative error in solving a spatially homogeneous problem using regression formulas for finding the energy-transition-rate coefficients relative to the direct use of formulas of SSH theory is 2%, a value which does not exceed the calculation error.

In a numerical study of the flow behind a shock wave, the following conditions in the free stream were considered: $T_0 = 300$ K, $\rho = 1.18 \times 10^{-4}$ kg/m$^3$, $p = 6.66$ Pa; the Mach number varied from 5 to 10. The populations of the vibrational levels were assumed to be equilibrium (Boltzmann distributions with the gas temperature $T_0$).

To validate the model, we compare the results obtained for M = 5 with those of [2], where calculations were carried out in the 4-temperature model using the MATLAB package (Fig. 5). The curves in the figure correspond to this study, and the symbols represent the results of [2]. It can be seen that the results are in good agreement. In addition, the figure shows the results obtained for a rougher two-temperature model
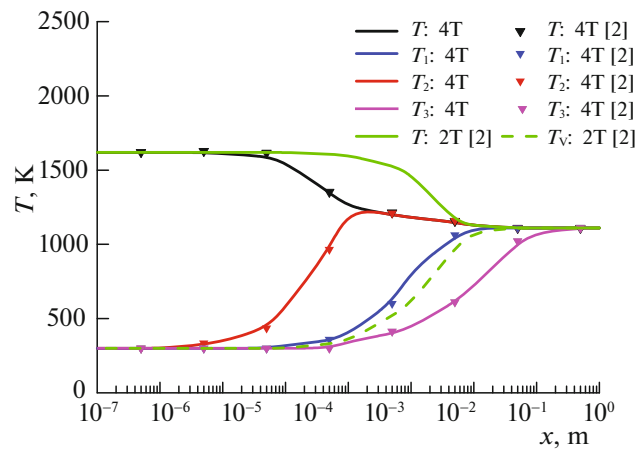
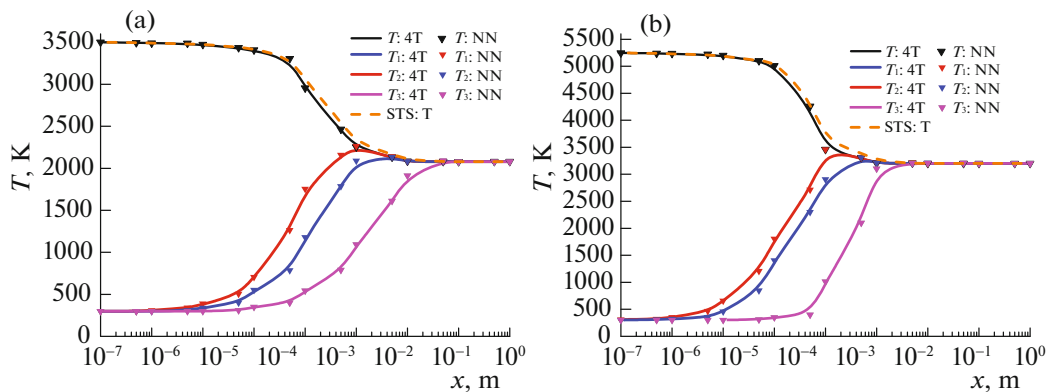**Fig. 5.** Temperature distribution behind the shock-wave front. M = 5. Comparison with the results of [2].



**Fig. 6.** Temperature distribution behind the shock-wave front at M = 8 (a) and M = 10 (b).

of vibrational relaxation in which the Landau–Teller formulas for relaxation terms are used [12]. The temperature distribution obtained in the two-temperature model is significantly different; relaxation begins noticeably later; and complete equilibrium is reached earlier. Since the two-temperature model does not take into account intermode energy exchanges, a conclusion can be made that these processes make a significant contribution to the character of relaxation behind shock waves.

Figure 6 shows the temperature distribution behind the shock-wave front at Mach numbers 8 and 10. Solutions are compared, which were obtained in the complete state-to-state approximation (STS), the hybrid multi-temperature approximation with the explicit calculation of relaxation terms (4T), and the multi-temperature approximation using neural networks (NN). For the state-to-state approximation, only the gas temperature $T$ is given. It is worth mentioning that the flow behind the shock wave in the complete state-to-state approximation has not been modeled in earlier studies. In all cases considered, the slowest process is the vibrational relaxation of the antisymmetric mode, and the fastest process is the relaxation of bending vibrations. As the temperature grows, the exchange rate increases, which leads to a rapid energy exchange between the first and second modes. Therefore, as the Mach number increases, the relaxation rates in these modes become close.

A comparison of the results showed that all considered approaches give close temperature distributions behind the shock wave, the average deviation from the reference state-to-state (STS) solution being 2.5–3%, and the maximum deviation being 4–6% for Mach numbers above 6. For smaller Mach numbers the maximum relative error is slightly higher (9%), but the absolute values of the relative errors are close for all test cases. The performance gain achieved in solving the problem turns out to be significant, which confirms that the use of multi-temperature models in combination with neural-network calculation of the relaxation rate is a promising approach.

**Table 1.** Efficiency in time of calculating relaxation terms ($TIME_R$), the time spent on the numerical method ($TIME_{num}$), and the total time for the solution of the system ($TIME_{sys}$) for complete state-to-state, hybrid 4T, and neural-network predicted 4T approaches in the problem of spatially homogeneous relaxation

| Approaches | $TIME_R$, s | $TIME_{num}$, s | $TIME_{sys}$, s |
|---|---|---|---|
| STS | 1130 | 370 | 1507 |
| 4T | 890 | 80 | 982 |
| NN | 65 | 80 | 148 |

**Table 2.** Efficiency in time of calculating relaxation terms ($TIME_R$), the time spent on the numerical method ($TIME_{num}$), and the total time for solution of the system ($TIME_{sys}$) for complete state-to-state, hybrid 4T, and neural-network predicted 4T approaches in the shock wave problem

| Approaches | $TIME_R$, s | $TIME_{num}$, s | $TIME_{sys}$, s |
|---|---|---|---|
| STS | 1214 | 1090 | 2310 |
| 4T | 1186 | 80 | 1270 |
| NN | 106 | 85 | 190 |

Table 2 compares the efficiency of solving the problem in the complete state-to-state approximation and the hybrid multi-temperature approximation with the explicit and neural-network methods for calculating relaxation terms. The time needed to calculate the relaxation terms is close to that in modeling spatially homogeneous kinetics. Nevertheless, the time spent on using the numerical method in the state-to-state approximation has increased by an order of magnitude, while for the hybrid model these figures are close. This is due to the high dimensionality of the system of equations, which greatly increases the computational complexity of solving systems of linear algebraic equations. The multi-temperature approach avoids this problem and is almost twice as efficient if relaxation terms are explicitly calculated and 12 times as efficient if neural networks are used. Therefore, with further complication of the problem, for example, in modeling a 2D or 3D flow, the advantages of using a hybrid approach and neural networks can additionally increase severalfold.

## 5. CONCLUSIONS

Various strategies for enhancing the efficiency of modeling $CO_2$ kinetics using machine-learning methods are considered. The application of neural networks to the direct solution of differential equations is shown not to yield the desired result. The most promising is the neural-network-based approach to calculating the rate of vibrational relaxation in a hybrid multi-temperature model: a spatially homogeneous problem has been solved more than an order of magnitude faster.

For the first time, the $CO_2$ flow behind a shock wave was simulated in the complete state-to-state approximation. The accuracy and efficiency of the obtained results was evaluated. A comparison is made with the results of other authors to show that the deviation of the obtained solutions does not exceed the calculation error. The hybrid 4-temperature approach, which uses the neural-network method for calculating relaxation terms, showed the best results in terms of time while maintaining the simulation accuracy. It is expected that in more complex two-dimensional and three-dimensional problems and in the case chemical reactions are taken into account, the gain will be even more significant.

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