

STATE-SPECIFIC TRANSPORT COEFFICIENTS WITH VARYING MOLECULAR DIAMETERS USING MACHINE LEARNING METHODS

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Abstract

One of the important issues in modern non-equilibrium gas dynamics is the correct modeling of all possible molecular distributions over internal energy levels, taking into account a varying collision diameter. This is important for the accurate calculation of physical properties, transport coefficients, and flux terms. In particular, it is significant for the modeling of thermal protection systems for re-entry spacecraft and hypersonic vehicles. This work is devoted to modeling various non-equilibrium vibrational distributions for molecular species that differ significantly from the well-known Boltzmann and Treanor distributions, taking into account the effect of varying collision diameters of vibrationally excited molecules. The obtained distributions are implemented in the problem of calculating state-specific transport coefficients, and, in particular, for the calculation of the thermal conductivity coefficient using machine learning methods. To accelerate the calculation speed, the developed accurate state-to-state approach is combined with different machine learning methods: linear regression, decision tree, random forest, as well as a neural network (multilayer perceptron). It is shown that, in terms of Shapley values for the neural network regression of thermal conductivity, the molar fraction of vibrationally excited states (taking into account the varying collisional diameter) is of the same order of magnitude as other input parameters. It is demonstrated that, in terms of generalization ability, the neural network represents the most appropriate technique.

Key words

Machine Learning (ML), Neural Network (NN), State-to-State Approach, Transport Coefficients, Varying Collision Diameter, Vibrational Distribution

1 Introduction

At present the state-to-state approach of the kinetic theory is one of the most accurate methods to describe strongly non-equilibrium gas flows. For high-speed flows, the effects of sharp temperature increases and physical and chemical non-equilibrium are observed. Under high-temperature non-equilibrium conditions, the internal degrees of freedom of atoms and molecules, as well as state-specific chemical reactions, play a significant role in real flow modeling issues [Nagnibeda and Kustova, 2009; Kunova et al., 2015]. Accounting for the effects of strong non-equilibrium is obligatory for the accurate calculation of heat and mass fluxes. These effects lead to aerodynamic heating of the surface and, therefore, must be taken into account very accurately. Detailed state-to-state non-equilibrium effects are associated with the excitation of internal degrees of freedom (in particular, vibrational and electronic), processes of dissociation and ionization, and state-specific chemical reactions [Istomin and Kustova, 2017b; Istomin and Kustova, 2017a; Istomin and Kustova, 2025].

For this reason, transport coefficients such as thermal conductivity and shear viscosity must be calculated very accurately. In modern engineering and applied physical problems, approximate semi-empirical formulae for calculation of transport coefficients are commonly used. Such formulae are validated within a narrow range of temperatures and pressures. The lack of accurate calculations of transport coefficients can lead to significant under- or over- estimation of heat fluxes, which in turn can impact the design of thermal protection for spacecraft or high-speed vehicles.

The state-to-state approach of the kinetic theory remains the most accurate and, simultaneously, the most

computationally expensive one. Under such an approach, the number of mixture species and, consequently, the number of equations for macroscopic parameters increases significantly (contrary to the simplest one-, two-, and multi-temperature approaches): each individual species represents a state with a specific energy and must be treated as an independent component of the mixture, with its own closed set of chemical state-specific reactions. The state-to-state approach is required when, in a gas mixture flow, the distribution over internal electronic-vibrational-rotational energy levels strongly deviates from the equilibrium distribution (realized in nozzles, high-speed flows, etc.).

A detailed algorithm for the calculation of transport coefficients under the vibrational state-to-state approach is considered in detail in [Nagnibeda and Kustova, 2009]. One of the key assumptions of such an approach is the independence of the elastic collision cross-section from the internal energy state of the colliding particles (specifically, the electronic-vibrational-rotational states of molecules), as well as from collisions leading to changes in internal states that vary in fast processes (determined by the gas dynamics time scale of the applied kinetic approach). Such a simplification allows the application of experimental data for the ground electronic-vibrational-rotational state of a molecule for the calculation of the collision integrals. However, such an assumption remains insufficiently rigorously justified.

Excitation of vibrational degrees of freedom for molecules leads to an increase in the effective collision diameter. A varying collision diameter may significantly affect collision integrals and, consequently, the calculated values of transport coefficients [Kustova and Kremer, 2015; Kornienko and Kustova, 2016; Istomin and Kustova, 2025; Istomin and Orlovskiy, 2026]. Meanwhile, at the present moment the influence of vibrational excitation on the collision diameter, and therefore on the transport coefficients remains poorly studied. In this regard, even the implementation of the vibrational state-to-state approach under strongly non-equilibrium conditions may not provide the required level of accuracy for the performed calculations.

Methods for calculating the effective collision diameters of electronic states of atoms and electronic-vibrational states of molecules are demonstrated in [Istomin and Kustova, 2017a; Istomin and Kustova, 2025]. In the paper [Istomin and Kustova, 2025], a vibrational-electronic state-to-state approach (STS-VE) for an electronically-vibrationally excited gas mixture of atoms and molecules is proposed: the additional simplified electronic state-specific approach (STS-E) assumes that relaxation of vibrational energy is a fast process, which significantly reduces the number of equations in the system for macroscopic parameters (relaxation of electronic energy is considered a slow process). Nevertheless, the influence of increasing collision diameters on the calculation of state-to-state transport properties remains poorly studied due to the computational com-

plexity of the problem.

The influence of a varying collision diameter of molecules coupled with the effect of a random distribution over vibrational states on transport coefficient calculation has been recently studied in [Istomin and Orlovskiy, 2026]. It is demonstrated that for molecular nitrogen N_2 , accounting for the varying collision diameter is important under conditions of strong vibrational non-equilibrium: for the state-specific thermal conductivity coefficient, it is significant at temperatures above 8000 K, while for shear viscosity, the effect is noticeable above 15000 K.

It is worth noting that accounting for the state-specific vibrational distribution coupled with the varying collision diameter effect is computationally demanding and time-consuming [Istomin and Orlovskiy, 2026]. Due to the computational complexity of the problem for accurate transport coefficient calculation, an assessment of applying machine learning algorithms for modeling is required. The present study aims to improve the accuracy of heat flux prediction in vibrationally non-equilibrium gas flows without a significant increase in computational complexity, as well as to speed up the calculation. Such an approach demonstrates novelty and potential demand for implementation in engineering applications [Istomin et al., 2023; Istomin and Pavlov, 2023]. The use of modern machine learning methods in engineering applications seems relevant due to their potential ability to approximate complex dependencies based on accurate research methods such as the kinetic theory approach. The application of neural network regressors and other machine learning algorithms can significantly reduce computational costs while maintaining acceptable accuracy. This is very important in many tasks involving multiple function calls for transport coefficient calculation, for example, in high-speed gas dynamics modeling, as well as in designing modern aerospace vehicles [Schmidt et al., 2019; Stokes et al., 2020; Brunton et al., 2020; Istomin and Kustova, 2021; Istomin and Pavlov, 2023; Istomin and Pavlov, 2025]. Such problems require transport calculations at each grid point and every time step, which makes the implementation of a time-consuming state-specific approach inappropriate. An overview and examples of machine learning implementation for modeling physical systems can be found in [Fradkov, 2022; Plotnikov et al., 2019; Fradkov and Shepeljavyi, 2022; Knyazev et al., 2023; Istomin and Pavlov, 2023], and, in particular, for the approximation of gas dynamics equations in computational fluid dynamics problems, as shown in [Ihme et al., 2009; Tracey et al., 2015; Sun et al., 2019].

It must be noted that neural networks have been used earlier for the calculation of transport coefficients: for example, for 11-component air flow under conditions of thermal and chemical equilibrium [You et al., 2023], for approximation of diffusion coefficients in binary mixtures [Kiva P., 2023], and in one-temperature [Istomin

and Pavlov, 2023] and two-temperature [Istomin and Pavlov, 2025] approaches of kinetic theory. The first attempt to evaluate the usability of a neural network for the problem of state-specific transport coefficient calculation is given in the paper [Istomin et al., 2023]. It was shown that the developed neural network architecture (multi-layer perceptron) is suitable with high accuracy for calculating the transport coefficients. At the same time, in that study, only the Boltzmann distribution over internal energy is considered and the effect of a varying collision diameter is neglected [Istomin et al., 2023; Istomin and Pavlov, 2023].

In the present study, for modeling purposes, molecular nitrogen N_2 is chosen as the main component of the Earth's and Titan's atmospheres. Also, results for N_2 are widely applied in various engineering applications. No electronic excitation is taken into account, as the main purpose of the work is to examine the influence of random vibrational distribution as well as varying collision diameters on the transport coefficient calculation procedure (the dependence on electronic-vibrational levels with varying collision diameters is planned to be studied in future works).

The present work is structured as follows: in the next section, the theoretical model for the calculation of state-specific transport coefficients, taking into account vibrational degrees of freedom, different distributions over vibrational levels (Boltzmann, Treanor, and random), and varying collision diameters, is provided; the third section shows the machine learning methods that are applied; the fourth section presents the results of the application of machine learning methods for a vibrationally excited flow of molecular nitrogen N_2 . Finally, the conclusion is provided.

2 Theoretical model

2.1 State-to-state approach

Based on the generalized Chapman–Enskog method, a self-consistent theoretical model of a non-equilibrium high-temperature gas mixture flow of neutral molecules and atoms, taking into account state-to-state kinetics of vibrational and electronic states of molecules, chemical reactions, ionization, and radiation, can be constructed [Kustova and Chikhaoui, 2000; Aliat et al., 2003; Nagnibeda and Kustova, 2009]. Within the present study, the state-specific effects associated with vibrational degrees of freedom are examined. The effects associated with the excitation of electronic degrees of freedom, ionization, and radiation are outside the scope of this work and may be the purpose of future studies. This approximation is named the state-to-state approach (hereafter referred to as STS) [Nagnibeda and Kustova, 2009].

Within the generalized Chapman–Enskog method, based on the relation between characteristic times of fast and slow processes, the system of governing equations is derived from the Boltzmann equation. The assumed relation between kinetic and gas-dynamic times makes

it possible to construct approaches with different levels of accuracy. In the present work, it is supposed that the following relation between characteristic times holds:

$$\tau_{tr} \lesssim \tau_{rot} \ll \tau_{vibr} < \tau_{react} \sim \theta, \quad (1)$$

here τ_{tr} , τ_{rot} , τ_{vibr} are the relaxation times for translational, rotational, and vibrational degrees of freedom, respectively; τ_{react} is the relaxation time of chemical reactions; θ is the fluid-dynamic time scale. According to relation (1), the gas represents a strongly non-equilibrium flow in terms of vibrational degrees of freedom and state-specific chemical reactions, coupled with fluid dynamics. For translational and rotational degrees of freedom, local equilibrium is assumed. Non-equilibrium conditions under relation (1) are observed, in particular, in nozzle flows, behind strong shock waves, etc. [Nagnibeda and Kustova, 2009].

Under the assumption (1), the set of governing equations for flow macroparameters can be written as follows:

$$\frac{dn_{c_i}}{dt} + n_{c_i} \nabla \cdot \mathbf{v} + \nabla \cdot (n_{c_i} \mathbf{V}_{c_i}) = R_{c_i}^{vibr} + R_{c_i}^{react}, \quad (2)$$

$$c = 1 \dots L, \quad i = 0 \dots L_c,$$

$$\rho \frac{d\mathbf{v}}{dt} + \nabla \cdot \mathbf{P} = 0, \quad (3)$$

$$\rho \frac{dU}{dt} + \nabla \cdot \mathbf{q} + \mathbf{P} : \nabla \mathbf{v} = 0, \quad (4)$$

here n_{c_i} is the number density of mixture components of species c on vibrational level i (for atoms the index i is omitted), ρ is the density, $\mathbf{v}$ is the gas velocity, $\mathbf{P}$ is the stress tensor, $\mathbf{q}$ is the heat flux vector, $\mathbf{V}_{c_i}$ is the diffusion velocity, L is the number of chemical species in the mixture, L_c is the number of vibrational levels for c -species, U is the total specific energy, $R_{c_i}^{vibr}$ and $R_{c_i}^{react}$ are the relaxation terms describing the vibrational (due to corresponding energy transitions; for atoms it is absent) and chemical reaction rates.

Within the Boltzmann equation, the description of non-equilibrium flow is based on the distribution function $f_{cij}(\mathbf{r}, \mathbf{u}, t)$ of mixture species c on vibrational i and rotational j energy levels of molecules as a function of velocity $\mathbf{u}$, coordinate $\mathbf{r}$, and time t . For atomic species only translational degrees of freedom are considered, and the distribution reduces to a Maxwell distribution over velocity.

The total specific energy per unit mass U , including the translational, rotational, and vibrational ones, as well as the specific formation energy, has the following form:

$$\rho U = \frac{3}{2}nkT + \sum_{c,i} \langle \varepsilon_{rot}^{c_i} \rangle n_{c_i} + \sum_{c,i} \varepsilon_i^c n_{c_i} + \sum_{c,i} \varepsilon_{form}^{c_i} n_{c_i}, \quad (5)$$

here $n = \sum_{c,i} n_{c_i}$ is the number density, k is the Boltzmann constant, T is the gas temperature, $\langle \varepsilon_{rot}^{c_i} \rangle$ is

the averaged rotational energy, ε_i^c is the vibrational energy, and $\varepsilon_{form}^{c,i}$ is the formation energy of species c on vibrational level i .

In the present study, the vibrational energy is calculated using the anharmonic oscillator model. Using the non-rigid rotator model, which takes into account the dependency on the vibrational level, the rotational energy is computed [Nagnibeda and Kustova, 2009]:

$$\begin{aligned} \langle \varepsilon_{rot}^{c,i} \rangle &= kT^2 \frac{\partial \ln Z_{c_i}^{rot}}{\partial T}, \\ Z_{c_i}^{rot}(T) &= \sum_j s_j^{c,i} \exp\left(-\frac{\varepsilon_j^{c,i}}{kT}\right), \end{aligned} \quad (6)$$

here $Z_{c_i}^{rot}$ is the rotational partition function, $s_j^{c,i}$ is the statistical weight of rotational level j , and $\varepsilon_j^{c,i}$ is the rotational energy.

Using the generalized Chapman-Enskog method, it is possible for each order of approximation to express the flux and relaxation terms in equations (2) – (4) via the macroparameters [Nagnibeda and Kustova, 2009]. In the first-order approximation of the modified Chapman-Enskog method, the following expressions for the stress tensor $\mathbf{P}$, diffusion velocity $\mathbf{V}_{c_i}$, and heat flux $\mathbf{q}$ can be obtained:

$$\mathbf{P} = (p - p_{rel} - \zeta \nabla \cdot \mathbf{v}) \mathbf{I} - 2\eta \mathbf{S}, \quad (7)$$

$$\mathbf{V}_{c_i} = - \sum_{d,k} D_{c_i d_k} \mathbf{d}_{d_k} - D_{T_{c_i}} \nabla \ln T, \quad (8)$$

$$\begin{aligned} \mathbf{q} &= -\lambda' \nabla T - p \sum_{c,i} D_{T_{c_i}} \mathbf{d}_{c_i} + \\ &\sum_{c,i} \left(\frac{5}{2} kT + \langle \varepsilon_{rot}^{c,i} \rangle + \varepsilon_i^c \right) n_{c_i} \mathbf{V}_{c_i} \end{aligned} \quad (9)$$

here p and p_{rel} are the pressure and relaxation pressure; η and ζ are the shear and bulk viscosity coefficients; $\mathbf{S}$ is the strain rate tensor; $\mathbf{I}$ is the unit tensor; $D_{c_i d_k}$ and $D_{T_{c_i}}$ are the diffusion and thermal diffusion coefficients for each chemical species c and d at vibrational levels i and k , respectively; $\lambda' = \lambda_{tr} + \lambda_{rot}$ is the thermal conductivity coefficient, consisting of two terms describing the contributions of translational and rotational degrees of freedom; $\mathbf{d}_{c_i}$ is the diffusion driving force for a particle of species c at vibrational level i :

$$\mathbf{d}_{c_i} = \nabla \left(\frac{n_{c_i}}{n} \right) + \left(\frac{n_{c_i}}{n} - \frac{\rho_{c_i}}{\rho} \right) \nabla \ln p. \quad (10)$$

It should be noted that under the state-to-state approach, the transport of vibrational energy is governed not only by thermal conductivity but also by the diffusion of vibrationally excited states [Kunova et al., 2015]. In shock-heated flows, the contribution of the diffusion of excited species to the heat transfer can be of the same

order of magnitude or even higher than that of classical mass diffusion. Coupling this fact with the sharply increasing number of equations for mass diffusion (the number of equations grows as the square of the number of mixture species, where each electron-vibrational state is treated as an individual species) leads to a high computational complexity of the problem. Therefore, for engineering applications, new, faster computational approaches are required. For these purposes, neural network regressors trained on precise calculation data are suitable, allowing for significant acceleration of state-specific calculations without loss of accuracy (see more details in the next section).

It should be noted that the aforementioned algorithm for the calculation of vibrationally state-specific transport coefficients and flux terms is implemented in the KAPPA software package [Campoli et al., 2019], and for the electronic-vibrational state-specific approach – in the PAINEt software package [Istomin and Oblapenko, 2018] (both packages are used in the present work). We refer the reader for details on the constructed algorithms for calculation of transport coefficients under state-to-state approaches, taking into account electron-vibrational excitation of molecules and electronic excitation of atoms, to the following studies [Istomin and Kustova, 2025; Istomin and Kustova, 2017a].

2.2 State-specific transport coefficients

Using the Chapman-Enskog method, the transport coefficients can be calculated. For the first-order distribution function, the reduction of integral equations to systems of linear algebraic equations is performed via expansions of the unknown functions into series of Sonine polynomials in peculiar velocity and Waldmann-Trübenbacher polynomials in internal energy [Ern and Giovangigli, 1994; Nagnibeda and Kustova, 2009].

Under the vibrational state-to-state approach, expressions for the thermal conductivity and thermal diffusion coefficients in terms of the expansion coefficients $a_{c_i, rp}$ have the following form:

$$\lambda' = \sum_{c,i} \frac{5}{4} k \frac{n_{c_i}}{n} a_{c_i,10} + \sum_{c,i} \frac{m_c}{2} \frac{n_{c_i}}{n} c_{rot,c_i} a_{c_i,01}, \quad (11)$$

$$D_{T_{c_i}} = -\frac{1}{2n} a_{c_i,00}, \quad (12)$$

here m_c is the mass of a particle of species c , c_{rot,c_i} is the specific heat of rotational degrees of freedom, i is the vibrational state.

The expressions for state-specific shear viscosity and mass diffusion coefficients in terms of the corresponding expansion coefficients $b_{c_i,r}$ and $d_{c_i,r}^{dm}$ have the following form:

$$\eta = \frac{kT}{2} \sum_{c,i} \frac{n_{c_i}}{n} b_{c_i,0}, \quad D_{c_i d_m} = \frac{1}{2n} d_{c_i,0}^{dm}. \quad (13)$$

Further, it is necessary to solve the systems of linear algebraic equations for the expansion coefficients. In the present study, we will focus on systems for thermal conductivity and shear viscosity coefficients, as they are the most commonly used in applied engineering applications.

The corresponding transport linear system of equations for $a_{ci,r}$ is used for computation of thermal conductivity as well as for thermal diffusion (can be found from the same system). Such a system has the form (14) and is supplemented by condition (15), which ensures the uniqueness of the solution:

$$\sum_{d,k} \sum_{r',p'} \Lambda_{rr'pp'}^{c_i d_k} a_{d_k,r'} = \frac{15kT}{2} \frac{n_{c_i}}{n} \delta_{r1} \delta_{p1} + 3m_c T \frac{n_{c_i}}{n} c_{\text{rot},c_i} \delta_{r0} \delta_{p1}, \quad (14)$$

$$c = 1 \dots L, \quad i = 0 \dots L_c, \quad r, p = 0, 1, \dots,$$

$$\sum_{c,i} \frac{\rho_{c_i}}{\rho} a_{c_i,0} = 0. \quad (15)$$

In the system above, $\Lambda_{rr'pp'}^{c_i d_k}$ is the bracket integral for species c and d on vibrational states i and k , correspondingly. Bracket integrals are generally expressed through the integral operator of fast processes and depend on elastic collisions and collisions leading to changes in internal energy in fast processes (in the present study - rotational energy, in accordance with relation (1)):

$$\Lambda_{rr'pp'}^{c_i d_k} = \sqrt{m_c m_d} \delta_{c_i d_k} \sum_{b,f} \frac{n_{c_i} n_{b_f}}{n^2} [\mathbf{Q}^{rp}, \mathbf{Q}^{r'p'}]_{c_i b_f}' + \sqrt{m_c m_d} \frac{n_{c_i} n_{d_k}}{n^2} [\mathbf{Q}^{rp}, \mathbf{Q}^{r'p'}]_{c_i d_k}'', \quad (16)$$

where $\mathbf{Q}^{rp}$ is the combination of Sonine and Waldmann-Trübenbacher polynomials of r and p order; the notations $[\dots]'$ and $[\dots]''$ correspond to partial bracket integrals [Nagnibeda and Kustova, 2009].

The shear viscosity η can be found using the same procedure as for the thermal conductivity coefficient. The first coefficient $b_{c_i,0}$ can be calculated from the following system:

$$\sum_{d,k} H_{00}^{c_i d_k} b_{d_k,0} = \frac{2}{kT} \frac{n_{c_i}}{n}, \quad (17)$$

$$c = 1 \dots L, \quad i = 0 \dots L_c,$$

here $H_{00}^{c_i d_k}$ is a bracket integral defined by fast processes, similarly to $\Lambda_{rr'pp'}^{c_i d_k}$ [Nagnibeda and Kustova, 2009].

The system for the calculation of mass diffusion coefficients can be found in [Istomin and Kustova, 2025].

2.3 Varying collision diameter

The omega integrals $\Omega_{cd}^{(l,r)}$ for species c and d on vibrational levels i and k are of importance for the calculation of bracket integrals. The omega integrals are expressed

using the averaging operator, which takes into account the form of the zero-order distribution function and contains the cross-section $\sigma_{cd,i,jkl}^{j'l'}$ of the most probable elastic collisions and collisions with rotational energy transitions.

The reduced omega integrals $\Omega_{cd}^{(l,r)*}$ are expressed as follows [Nagnibeda and Kustova, 2009]:

$$\Omega_{cd}^{(l,r)*} = \frac{\Omega_{cd}^{(l,r)}}{\left(\Omega_{cd}^{(l,r)}\right)_{\text{r.s.}}}, \quad (18)$$

$$\left(\Omega_{cd}^{(l,r)}\right)_{\text{r.s.}} = \left(\frac{kT}{2\pi m_{cd}}\right)^{1/2} \frac{(r+1)!}{2} \left(1 - \frac{1 + (-1)^l}{2(l+1)}\right) \pi \sigma_{cd}^2, \quad (19)$$

here $\left(\Omega_{cd}^{(l,r)}\right)_{\text{r.s.}}$ is the omega integral of the rigid sphere model; $\sigma_{cd} = (\sigma_c + \sigma_d)/2$ is the distance between the centres of molecules c and d with collision diameters σ_c and σ_d [Nagnibeda and Kustova, 2009]. Contrary to omega integrals, reduced omega integrals have a weaker dependence on temperature, and are usually close to unity. This last fact makes them widely used in practical calculations.

It is typically assumed that the collision diameter and scattering angle do not depend on the vibrational level of the colliding particles: $\Omega_{cd,i,k}^{(l,r)} = \Omega_{cd}^{(l,r)}$. However, for real flows this relation may not be satisfied. In the present study, this assumption is neglected because the collision diameters of vibrationally excited molecules σ_{c_i} and σ_{d_k} are calculated directly using the Morse model [Gordillo-Vazquez and Kunc, 1998] as a special case of the Tietz-Hua model [Kunc and Gordillo-Vazquez, 1997; Gorbachev et al., 1997]:

$$\sigma_{c_k - c_k} = r_{c_k} + 2.3 \text{ \AA}, \quad k = (n, i, j), \quad (20)$$

$$r_{c_k} = r_e(n) + \beta^{-1} \ln \left(\frac{\phi_2 + 2\sqrt{\phi_1 \phi_3}}{-4\phi_3 \text{sign}(\phi_2)} \right), \quad (21)$$

here β is the Morse constant for molecules of species c on the electron-vibrational-rotational level (n, i, j) ; ϕ_1, ϕ_2, ϕ_3 are calculated coefficients [Gordillo-Vazquez and Kunc, 1998].

The use of the Tietz-Hua and Morse models yields close values for the calculated diameters [Kornienko and Kustova, 2016; Istomin and Kustova, 2025; Istomin and Orlovskiy, 2026], but the Morse model is computationally simpler. In the present study, the Morse model is applied for molecules in the ground electronic state and without the contribution of rotational excitation on the collision diameter. In Figure (1), the calculated dependencies of N_2 , NO , and O_2 collision diameters on the

vibrational (i) and fixed rotational ($j=0,100$) levels are given (the ground electronic energy level is considered). It is clearly seen that the impact of rotation on the collision diameter increases only for the rotationally excited high-lying vibrational states. Such states are usually underpopulated, and very close to the dissociation energy limit. In the present study, we will not take into account this effect and it can be studied in future investigations. The possibility of such an assumption in the ground electronic state is also discussed in [Istomin and Kustova, 2025].

In this case, the triplet (n, i, j) in formula (20) reduces to a single index i . Dimensional collision integrals are obtained by multiplying the reduced collision integrals [Bruno et al., 2008] by the omega integral of the rigid sphere model. Details of the algorithm for accounting for the varying collision diameter can be found in [Istomin and Kustova, 2025]. Further, we will refer to STS-VD as the STS approach taking into account varying collision diameters.

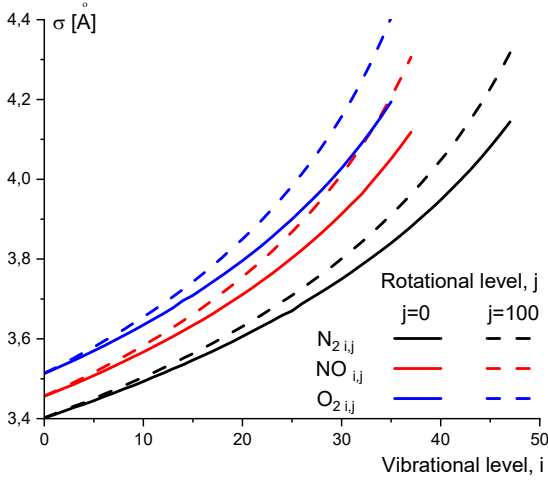


Figure 1. Dependencies of N_2 , NO , and O_2 collision diameters on the vibrational (i) and fixed rotational ($j=0,100$) levels.

2.4 Different vibrational distributions

For strongly non-equilibrium gas mixture flows, the vibrational distribution may not satisfy the well-known and usually used Boltzmann and Treanor distributions. The Boltzmann distribution is the equilibrium distribution under the one-temperature approach, and the Treanor is the distribution with a vibrational temperature that differs from the gas temperature (the so-called two-temperature approach). The Boltzmann distribution over vibrational energy levels is represented by the following formula:

$$n_{ci} = \frac{n_c}{Z_c^{vibr}} s_i^c \exp\left(-\frac{\varepsilon_i^c}{kT}\right), \quad (22)$$

$$Z_c^{vibr}(T) = \sum_i s_i^c \exp\left(-\frac{\varepsilon_i^c}{kT}\right),$$

here Z_c^{vibr} is the vibrational partition function, s_i^c is the statistical weight of vibrational level i .

The Treanor vibrational distribution can be calculated using the following relation:

$$n_{ci} = \frac{n_c}{Z_c^{vibr}(T, T_1^c)} s_i^c \exp\left(-\frac{\varepsilon_i^c - i\varepsilon_1^c}{kT} - \frac{i\varepsilon_1^c}{kT_1^c}\right), \quad (23)$$

$$Z_c^{vibr}(T, T_1^c) = \sum_i s_i^c \exp\left(-\frac{\varepsilon_i^c - i\varepsilon_1^c}{kT} - \frac{i\varepsilon_1^c}{kT_1^c}\right),$$

here T_1^c is the temperature of the first vibrational level of species c , ε_1^c is the energy of the first vibrational level of species c .

For specifying a random distribution over vibrational levels, we will use the Boltzmann and Treanor distributions as the upper and lower limits $[a, b]$. Such an approach ensures the physicality of such distributions in high-speed gas dynamic problems [Istomin and Orlovskiy, 2026]. For the random distribution, we will use the approach proposed in [Istomin and Orlovskiy, 2026]:

$$x = \alpha \cdot x_{tri} + (1 - \alpha) \cdot x_{log}, \quad \alpha = 0.5. \quad (24)$$

In equation (24), the generated value x is computed as a superposition of the triangular x_{tri} and lognormal x_{log} distribution values. Such an approach ensures the diversity (triangular distribution) and specificity (lognormal distribution) of the generated vibrational population values, as well as keeping the physically allowed distribution limits.

In Figure 2, two examples of the constructed random distributions are shown. In the top figure, the condition of weak vibrational excitation $T > T_1$ ($T = 4907$ K, $T_1 = 4221$ K) is represented; in the bottom figure, an example of a strongly vibrationally excited flow $T \leq T_1$ ($T = 17563$ K, $T_1 = 19665$ K) is demonstrated. It is clearly seen that from a numerical point of view, the discrepancies in the molar fractions of excited vibrational states in application to the state-to-state approach may lead to various results for the calculated transport coefficients and flux terms. Moreover, the complexity of the problem becomes extremely high when coupled with the effect of a varying collision diameter for each vibrationally excited state. Under such conditions, the implementation of methods like machine learning becomes highly desirable.

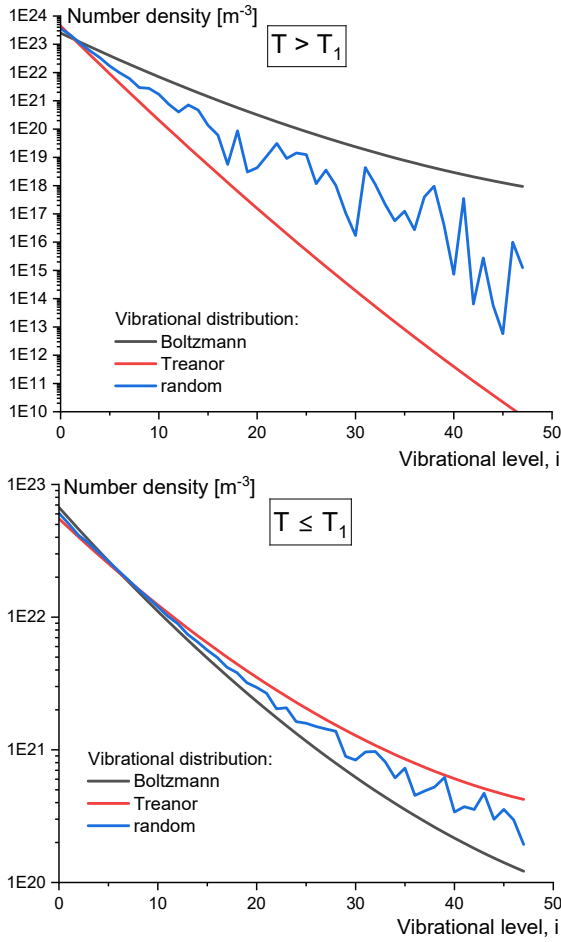


Figure 2. Examples of different distributions over N_2 vibrational levels for cases of weak $T > T_1$ (upper figure; $T = 4907$ K, $T_1 = 4221$ K) and strong $T \leq T_1$ (lower figure; $T = 17563$ K, $T_1 = 19665$ K) vibrational non-equilibrium.

3 Application of machine learning methods

In the present study, a machine learning regression model is constructed according to the following scheme:

$$[T, T_1, p, n_1, \dots, n_k] \rightarrow \lambda. \quad (25)$$

For an input vector consisting of 51 components (temperature T , temperature of the first vibrational level T_1 , pressure p , and molar fractions $n_1, \dots, n_k$ of 48 vibrational states of molecular nitrogen N_2), a regression is performed for the output quantity, which represents the thermal conductivity coefficient λ . In the general case, the output value can also be a vector, for example, containing components with some physical properties, other transport coefficients, etc. Results for such an implementation for the regression of an output vector can be found in papers [Istomin and Pavlov, 2023; Istomin and Pavlov, 2025]. In the given study, for simplicity of calculations, we limit ourselves to the scalar quantity λ , whose calculation for the training dataset is performed using the STS-VD approach, taking into account the effect of different distributions over vibrational levels and varying

collision diameters. The choice of thermal conductivity λ instead of the pair of values (λ, η) will be discussed in the next section.

The input data consists of randomly generated vectors with values taken from uniform distributions within the following ranges: for temperatures $T = 293 - 20000$ K, $T_1 = 293 - 35000$ K; pressure $p = 300 - 100000$ Pa, and a dataset of random molar fraction distributions. The dataset is split into train/test/valid sub-datasets by the following proportion: 81/9/10%.

It is well known that for a regression problem, the usual statistical method like naive linear regression is ineffective at handling complex interactions within the dataset. Contrary to this, the implementation of machine learning methods makes it possible to increase generalization ability. As a typical set of usual machine learning methods, we consider linear regression, decision trees, and one of the ensemble methods - random forest. It must be emphasized that the implementation of these algorithms is associated with the generation of large datasets for effective model training.

Table 1. Machine learning algorithms and optimal hyperparameters

Algorithm	Optimal parameters
Linear regression	with intercept
Regression tree	depth: up to 500
Random forest	depth: up to 100 number of trees: 500
Neural network (multilayer perceptron)	number of hidden layers: 1 number of neurons per layer: 64 pre-trained number of epochs: 3 fine-tuned number of epochs: 4 activation function: tanh batch size: 128 pre-trained learning rate : 0.01 fine-tuned learning rate : 0.0001 pre-trained directed dropout : saturation ≥ 0.9 fine-tuned directed dropout : saturation ≥ 0.85

For the training procedure, two datasets are generated. The first dataset is created following scheme (25) and is used for every method. The second dataset is used only for the neural network pre-training stage. It includes an additional component, λ_{1T} (the thermal conductivity from a one-temperature approach), effectively making the input vector $[T, T_1, p, n_1, \dots, n_k, \lambda_{1T}] \rightarrow \lambda$, serving as a kind of transfer learning technique. The realization

of two-stage (pre-training and fine-tuning) helps the neural network to associate the output state-specific thermal conductivity value more closely with the real flow range of thermal conductivity values, calculated with a computationally simple one-temperature approach. Also, this approach allows for a reduction in the number of training epochs. All other models are trained only on the first dataset.

The performance quality of the algorithms is evaluated using the following metrics: MSE (Mean Squared Error), MAE (Mean Absolute Error), R^2 (coefficient of determination). Additionally, the average execution time for the learning (t_{learn}) and prediction (t_{pred}) steps is analyzed.

For the regression problem, the machine learning methods are taken from the scikit-learn library [Pedregosa et al., 2011]. Our previous research has shown the effectiveness of neural network regressors (multi-layer perceptron) compared to other regression methods due to their significant flexibility and computational efficiency for the considered type of problem [Istomin and Pavlov, 2023; Istomin and Pavlov, 2025]. Nevertheless, since for the present case the output vector represents a scalar unit, it may be possible to find that other machine learning methods show higher computational efficiency.

The hyperparameters of the applied methods are shown in Table 1. It is worth noting that due to the complexity of the neural network learning, we reduced the number of training epochs significantly by using some specific techniques: separation of training into two stages of pre-training and fine-tuning; supplementation of additional information on λ_{1T} (see discussion above); applying directed dropout for neurons with a high value of saturation; reduction of the learning rate for the fine-tuning stage, etc. Such an approach helps to maintain the generalization ability of the network, which is of importance for the current problem.

The hyperbolic tangent is used as the activation function: $\tanh(x) = (e^x - e^{-x}) / (e^x + e^{-x})$. It has been shown that the $\tanh(x)$ function is more suitable for regression of smooth functions [De Ryck T., 2021]. For the training procedure, the Adam optimizer [Kingma D., 2014] is chosen. During the training, the MSE metric is used as a loss function.

For interpretation ability, the Shapley model is implemented for all trained machine learning methods [Shapley, 1951]. In the context of machine learning, the Shapley value for some feature is defined as the average contribution of an individual feature to the change in the prediction of a model across all possible subsets of features. Thus, the Shapley value allows us to estimate the importance of each individual feature for the result of the regression given by a neural network. During the training, the contribution of each input vector feature in terms of Shapley values is performed.

For the numerical experiments, a personal computer with the following characteristics was used: AMD Ryzen 7 5800 8-Core Processor 3.40 GHz, NVIDIA

GeForce RTX 3060 video card, MPG B550 GAMING PLUS (MS-7C56) motherboard, RAM 32 Gb.

4 Results

4.1 Transport coefficients

The thermal conductivity λ and shear viscosity η coefficients for state-specific molecular nitrogen N_2 as a function of temperature under different kinetic approaches are given in Figures 3 and 4. The state-specific calculation of λ taking into account the Treanor distribution (STS) for a vibrationally excited flow ($T = 1.75T_1$), and varying collision diameter (STS-VD) was carried out in the KAPPA software package [Campoli et al., 2019]. The calculation of state-specific η taking into account the Boltzmann distribution (STS) and varying collision diameter (STS-VD) was performed in the *PAINeT* software package [Istomin and Oblapenko, 2018].

It is clearly seen that both figures look very similar: the influence of the varying diameter coupled with different distributions over vibrational levels becomes about 3-5% at temperatures in the range of 10000 - 15000 K, but for thermal conductivity, the impact of the effects becomes noticeable starting at 8000 K. Taking into account this last fact, and due to the similar behavior of the thermal conductivity λ and shear viscosity η coefficients in terms of the discrepancy growth between the STS and STS-VD approaches, in the further machine learning modeling we will focus on the regression of one of these coefficients, λ .

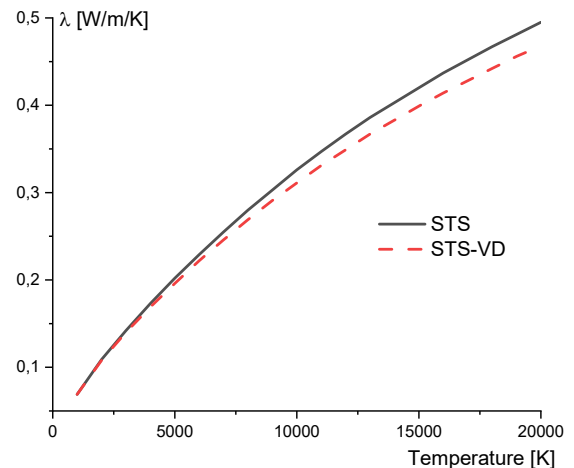


Figure 3. Thermal conductivity λ of N_2 as a function of temperature for different kinetic approaches with the Treanor distribution $T_1 = 1.75T$.

4.2 Optimal neural network regression model

In Table 2, the metric results for different machine learning regressions of thermal conductivity are pre-

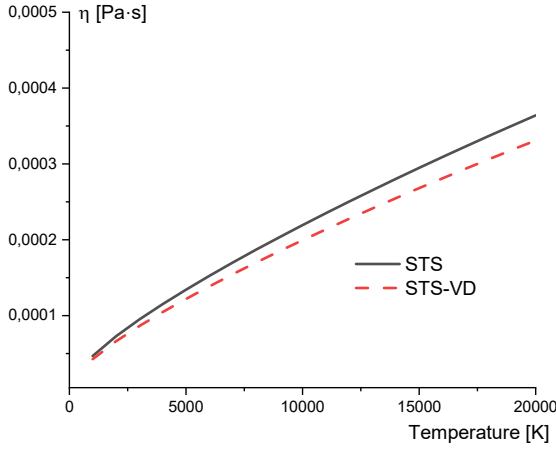


Figure 4. Shear viscosity η of N_2 as a function of temperature for different kinetic approaches with the Boltzmann distribution.

Table 2. Comparison of accuracy metrics for N_2 regression of state-specific λ .

Algorithm	MSE	MAE	R^2
Linear regression	0.003	0.012	0.996
Regression tree	2e-7	0.0008	0.999
Random forest	6e-8	0.0005	0.999
Pre-trained neural network	0.036	0.156	0.449
Fine-tuned neural network	0.003	0.04	0.95

sented. It is shown that for linear regression, decision tree, and random forest, the quality of all metrics MSE, MAE, and R^2 is very high, and the quality increases with the complexity of the method. At the same time, the evaluation of these methods on the basis of Shapley values shows that the impact of the first feature of the input vector (temperature T) is several orders of magnitude higher than other features like molar fractions. Therefore, no out-of-sample performance for the state-specific transport coefficient can be achieved from these kinds of models.

Due to the last fact, the neural network (multilayer perceptron) was chosen as the most promising approach for high out-of-sample performance. Earlier, it was shown that the neural network can be very quickly trained on the first dataset to the best values of metrics as for linear regression, decision tree, and random forest (for example, see our previous research [Istomin and Pavlov, 2023; Istomin and Pavlov, 2025]). While our purpose is to achieve the maximum of predictive accuracy for the STS-VD approach, as well as to obtain some information on the contribution of different vibrational levels (varying collision diameters) to the resulting value of λ , we use for the neural network the transfer learning technique by separating the training procedure into two stages: pre-training and fine-tuning. In the pre-training stage we use an additional input neuron to show the net-

work what is the typical range of λ_{1T} values for a specific initial condition with temperature T , pressure p , and molar fractions that correspond to the Boltzmann distribution. In the second stage, we removed this information and fine-tuned the network on the "typical" for all models dataset. During the training, the directed dropout is applied for neurons with a saturation of at least 0.85 in absolute value (0.9 for the pre-training stage). Such an approach allows us to considerably decrease the number of training epochs as well as to preserve generalization ability. The out-of-sample performance is achieved by maintaining the same order of Shapley values for all the input vector features (in other words, their "influences").

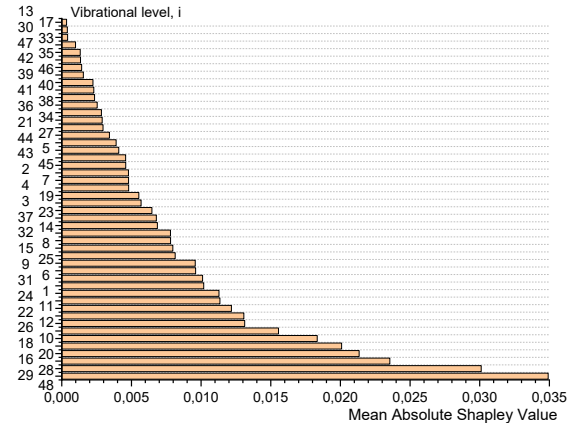


Figure 5. Ranked list of mean absolute Shapley values for each vibrational level (i) of N_2 .

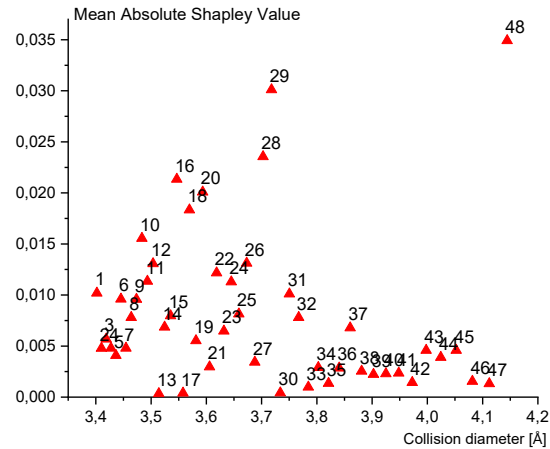


Figure 6. Mean absolute Shapley value of each vibrational level of N_2 as a function of collision diameter.

For the fine-tuned neural network, the accuracy metrics achieved the following values: the MSE is equal to that of the linear regression model, but the coefficient of

determination R^2 is worse by approximately 0.05 points than the R^2 of the other models. At the same time, an R^2 value of 0.95 remains a very good result in terms of regression ability. Therefore, the fine-tuning of the neural network on the basis of Shapley values being of the same order of magnitude leads us to a compromise with slightly worse training results on the metrics. At the same time, we achieved the ability to analyze the logic of the neural network regression in terms of the state-to-state approach.

In Figures 5 and 6, the impact of different vibrational levels in terms of Shapley values is given. Following the results of Figure 5, it can be concluded that the most influential vibrational states according to the Shapley method correspond to the high-lying vibrational levels and, therefore, to the maximum collision diameters. Additional analysis presented in Figure 6 shows that for the entire set of vibrational levels, there is no direct correlation between the mean absolute Shapley values and the varying collision diameter value. Therefore, we can suggest the absence of a linear relationship between these features in the constructed model and the regression result. We can conclude that the slightly worse performance in terms of calculation metrics, coupled with the high generalization ability, represents a generalized model for the STS-VD approach. Due to the balanced influence of input features, it helps to take into account the non-equilibrium effects.

Table 3. Comparison of training t_{learn} and prediction t_{pred} times for N_2 regression of state-specific λ .

Algorithm	$t_{learn}, [s]$	$t_{pred}, [s]$	$\frac{t_{learn}}{t_{pred}}$
Linear regression	96	1	96
Regression tree	4317	2	2159
Random forest	43187	40	1080
Pre-trained neural network	2271	1	2271
Fine-tuned neural network	4486	1	4486

In Table 3, the comparison of the training t_{learn} and prediction $t_{predict}$ times for different machine learning methods is given. The additional metric in the table, $t_{learn}/t_{predict}$ allows us to assess the efficiency trade-off between the learning and prediction stages. As can be seen from the Table 3, the execution time for calculation of the output feature for the neural network is comparable to the results of the regression tree, and outperforms the result of the random forest. For the given first dataset of λ under STS-VD approach (see (25)), the speed-up in calculation time between KAPPA and the neural network shows an increase in performance of about 34,000 times. This last result opens great opportunities for future development of such a calculation approach.

5 Conclusion

In the present study, the STS and STS-VD kinetic approaches for the calculation of state-specific transport coefficients, taking into account vibrational degrees of freedom, different vibrational distributions (Boltzmann, Treanor, and random), and varying collision diameters, are provided. The behavior of varying collision diameters of the ground electronic states of molecules N_2 , NO , and O_2 on the vibrational and rotational levels is shown. The method of physically adequate random vibrational distribution generation is discussed. The results of applying the STS and STS-VD approaches to the calculation of transport coefficients of thermal conductivity and shear viscosity are given.

The developed models are used to generate two databases for training different machine learning algorithms: linear regression, decision tree, random forest, and neural network (multilayer perceptron). The regression of the thermal conductivity coefficient of a vibrationally excited flow of molecular nitrogen N_2 with varying collision diameters is examined. For training the neural network, seeking to maintain generalization ability, two-stage transfer learning is implemented. It is shown that while the constructed neural network is slightly worse in terms of MSE and R^2 metrics compared to other machine learning methods, its opportunity to be an out-of-sample regressor in terms of Shapley values makes it an even better decision for application to engineering problems. During the training of the neural network for the thermal conductivity regression, all input vector features, including the molar fraction of vibrationally excited states with varying collisional diameter, were learned to be of the same order of magnitude in terms of Shapley values. This fact leads us to the conclusion that the model has a high generalization ability for out-of-sample calculation performance. Due to the balanced influence of input features, the constructed neural network regressor allows us to take into account and analyze the non-equilibrium effects. Moreover, the speed-up between accurate calculation based on the kinetic approach and the neural network regression achieves a value of 34,000 times.

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