

# State-resolved models of chemical reactions for non-equilibrium flow simulations

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## Abstract

In this paper, the assessment of existing theoretical models for the vibrational state-resolved Zeldovich exchange reaction is carried out on the basis of comparison with the results of several quasi-classical trajectory (QCT) calculations. An error in the theoretical model proposed by Aliat is corrected; after correction this model provides a very good agreement with the QCT reaction rate coefficients. Then the model is further generalized in order to take into account the vibrational state of the reaction product, namely, of the NO molecule which is formed as a result of the Zeldovich reaction. The generalized rate coefficients are in fairly good agreement with the QCT results in the whole range of temperatures and vibrational states of both reagents and products. Using the non-equilibrium Boltzmann distribution we study the multi-temperature reaction rate coefficients, obtained by averaging the state-specific ones. The effect of the vibrational temperature of the reaction product is evaluated. It is shown that variation of the NO vibrational temperature does not affect significantly the rate coefficients. Thus both commonly used assumptions that NO molecules are produced either in thermal equilibrium or in the ground state are valid for simulations of non-equilibrium high-temperature flows.

## 1. Introduction

Theoretical simulations of high-temperature non-equilibrium flows typical in planetary entry problems require detailed models for collisional processes in gases under consideration. Molecular dynamics provides accurate data for the cross sections and rate coefficients of physical and chemical processes. However these data cannot be directly applied in the computational fluid dynamics (CFD) due to considerable computational efforts required for their implementation. Moreover existing approximations obtained on the basis of trajectory calculations have a limited range of applicability and are closely associated with the used vibrational ladder and therefore cannot be easily transferred to other models. At the same time, for the description of state-to-state kinetics, a fairly simple model for the reaction rate coefficients based on the Treanor-Marrone model<sup>9</sup> can be applied.

Previously, we have developed simple but accurate models for the state-resolved dissociation rate coefficients<sup>7,8,14</sup> based on the comparison with quasi-classical trajectory calculations (QCT).<sup>2,5,6,11</sup> Piecewise continuous functions for the Treanor-Marrone model parameter  $U$  in  $O_2/O$  and  $N_2/N$  mixtures depending on the temperature and the vibrational energy state have been obtained by fitting the rate coefficients to those given by the QCT calculations. One of the significant advantages of the proposed model is its independence of the vibrational ladder. The results obtained using these models demonstrate a very good agreement with the QCT calculations. The models were used to simulate binary  $O_2$  and  $N_2$  mixture flows as well as air flows behind the shock wave.<sup>8</sup>

At the same time, the exchange reaction rate coefficients are not very well studied up to now. There are only a few models depending on the vibrational level, for instance the Warnatz model,<sup>16</sup> approximations of trajectory calculations for the first 30 levels of  $N_2$  and 15 levels of  $O_2$ ,<sup>3</sup> and a theoretical generalization of the Treanor-Marrone model.<sup>1</sup> Some data are also available in the STELLAR database.<sup>15</sup>

The main idea of this work is to provide a range of parameters for the generalised Treanor-Marrone-like model for the state-resolved exchange reaction rate coefficients. In particular, we study the Zeldovich reaction



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where  $i$  and  $k$  are the vibrational states of corresponding molecules. A method similar to that described in<sup>7</sup> allows us to obtain the sought parameters as functions of temperature and vibrational energy of both the reaction reagents and products and thus to get the state-specific exchange reaction rate coefficients close to those given by QCT calculations. The resulting model with variable parameters retains the simplicity and structure of the original model but provides much better accuracy.

Based on the developed state-resolved model we calculate two-temperature exchange reaction rate coefficients using the non-equilibrium Boltzmann vibrational distributions and compare to the existing models. The effect of the reaction product vibrational temperature on the exchange reaction rate is evaluated.

All the developed models can be easily integrated into the CFD and used in simulations of strongly thermochemically non-equilibrium flows.

## 2. State-resolved exchange reactions rate coefficients models

We have examined the existing theoretical models of the rate coefficients for non-equilibrium exchange reactions and compared them with those obtained by means of quasi-classical trajectory calculations (QCT). The following models are considered:

1. The Rusanov-Fridman model<sup>13</sup> taking into account the efficiency of the vibrational energy contribution to the activation energy. The exchange reaction rate coefficients in this case are written as:

$$k_{N_2i,O}^{exch}(T) = A(T) \exp \left[ -\frac{E_a - \alpha \varepsilon_i^{N_2}}{kT} \Theta(E_a - \alpha \varepsilon_i^{N_2}) \right], \quad (2)$$

where  $\alpha$  is the vibrational energy efficiency coefficient,  $\Theta$  is the Heaviside step function,  $E_a$  is the reaction activation energy. The pre-exponential factor  $A(T)$  is approximately equal to the collision frequency at a single concentration  $A(T) \approx \pi r_0^2 (8kT/\pi\mu)^{1/2}$ ,  $r_0$  is the gas-kinetic collision radius,  $\mu = m_1 m_2 / (m_1 + m_2)$  is the reduced mass,  $\alpha = 0.51$ .

2. The Polak's model<sup>12</sup> based on the approximation of trajectory calculations:

$$k_{N_2i,O}^{exch}(T) = A(T) \exp \left[ -\frac{E_a - \gamma \varepsilon_i^{N_2}}{\beta kT} \Theta(E_a - \gamma \varepsilon_i^{N_2}) \right], \quad (3)$$

here  $A(T)$  is defined similarly to the Rusanov-Fridman model, and the parameters  $\beta = 0.9$  and  $\gamma = 0.52$  characterize the contributions of translational and vibrational energies into the reaction.

3. Based on the chemically activity collisions theory, Warnatz proposed his own model<sup>16</sup> for the exchange reactions rate coefficients:

$$k_{N_2i,O}^{exch}(T) = C(i+1)T^\beta \exp \left[ -\frac{E_a - \varepsilon_i^{N_2}}{kT} \Theta(E_a - \varepsilon_i^{N_2}) \right], \quad (4)$$

in the case of  $N_2+O$  collision the following values of parameters are used:  $C = 4.17 \cdot 10^{12}$ ,  $\beta = 0$ .

4. An approach based on the generalization of the Treanor-Marrone method with allowance for electronic excitation was proposed by A. Aliat.<sup>1</sup> In the particular case of the ground electronic state it turns into the model that depends only on the vibrational level. Then the exchange reaction rate coefficients are calculated as follows:

$$k_{ci,d}^{exch}(T, U) = \begin{cases} C(T, U) k_{eq}^{exch} \exp \left( -\frac{E_a}{kU} \right) \exp \left[ \frac{\varepsilon_i^c}{k} \left( \frac{1}{T} + \frac{1}{U} \right) \right], & \varepsilon_i^c < E_a \\ C(T, U) k_{eq}^{exch} \exp \left( \frac{E_a}{kT} \right), & \varepsilon_i^c > E_a, \end{cases}, \quad (5)$$

where  $T$  is the temperature,  $U$  is the Treanor-Marrone model parameter,  $k$  is the Boltzmann constant,  $k_{eq}^{exch}$  is the thermal equilibrium rate constant of the exchange reaction:

$$k_{eq}^{exch} = AT^b \exp \left( -\frac{E_a}{kT} \right), \quad (6)$$

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$A$ ,  $b$  are the parameters found by fitting experimental data,  $E_a$  is the reaction activation energy,  $\varepsilon_i^c$  is the vibrational energy of the molecule  $c$  at the corresponding level, the normalizing coefficient  $C(T, U)$  is calculated by the expression:

$$C(T, U) = \left[ \sum_{i(1)} \frac{1}{Z_c^{vibr}(T)} \exp\left(-\frac{E_a - \varepsilon_i^c}{kU}\right) + \sum_{i(2)} \frac{1}{Z_c^{vibr}(T)} \exp\left(-\frac{E_a - \varepsilon_i^c}{kT}\right) \right]^{-1}, \quad (7)$$

where  $Z_c^{vibr}(T)$  is the equilibrium vibrational partition function, (1) =  $\varepsilon_i^c < E_a$ , and (2) =  $\varepsilon_i^c > E_a$ . Calculations for this model are performed using two classical parameter  $U$  values:  $U = 3T$  and  $U = D/6k$ . For  $N_2+O$  reaction,  $E_a = 5.175 \cdot 10^{-19}$  J or 3.23 eV,  $A = 0.8 \cdot 10^{-16}$  m<sup>3</sup>/s,  $b = 0$ .

The exchange reaction rate coefficients were calculated for the all presented models using the anharmonic oscillator model for the vibrational levels of the reacting molecule in the temperature range from 2000 K to 20,000 K with the increment of 1000 K. The results are compared with the data from the Stellar<sup>15</sup> database, which presents the results of QCT calculations for chemical reactions in air (using its own ladder of vibrational levels). It is worth mentioning that all above theoretical models do not take into account the vibrational state of the reaction product, namely, the NO molecule. Therefore for the comparison with the QCT data, the rate coefficients corresponding to the case of NO formation at the ground state ( $k=0$ ) are chosen from the database. The rate coefficients as functions of the  $N_2$  vibrational energy for fixed temperatures are shown in Fig. 1, and in Fig. 2 they are given as functions of temperature at fixed vibrational levels.

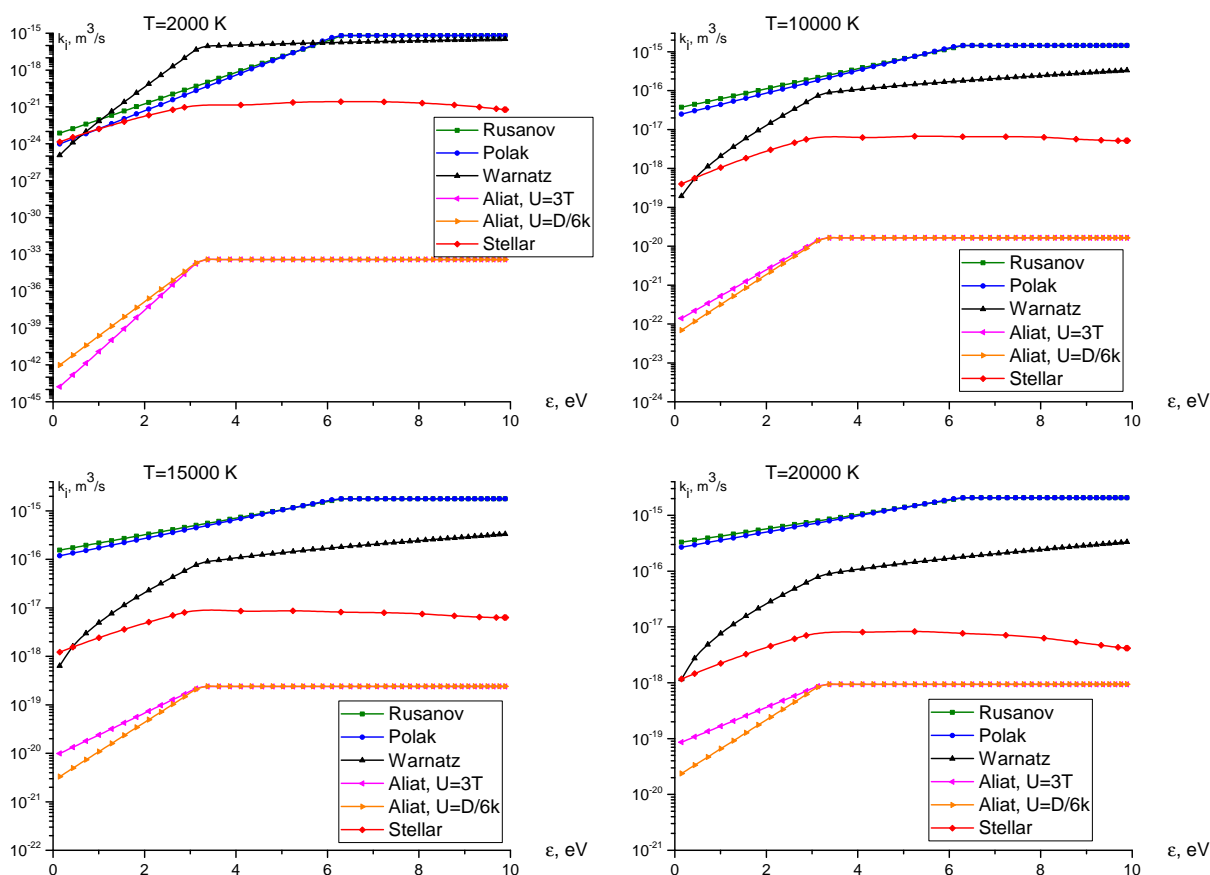


Figure 1: Exchange reaction rate coefficients for  $N_2+O$  reaction as functions of the  $N_2$  vibrational energy with fixed temperature for different models.

It is seen from the Fig. 1 that the coefficients obtained using the Rusanov-Fridman, Polak, and Aliat models show the following feature: starting from a certain vibrational level (determined by the combination of the activation energy and parameters which characterize the contributions of translational and vibrational energies into the reaction), the growth of the coefficients at a given temperature ceases, and they attain the constant value. Contrarily, the use of the Warnatz formula provides a slow but steady increase in the coefficients in the whole range of vibrational levels. At the

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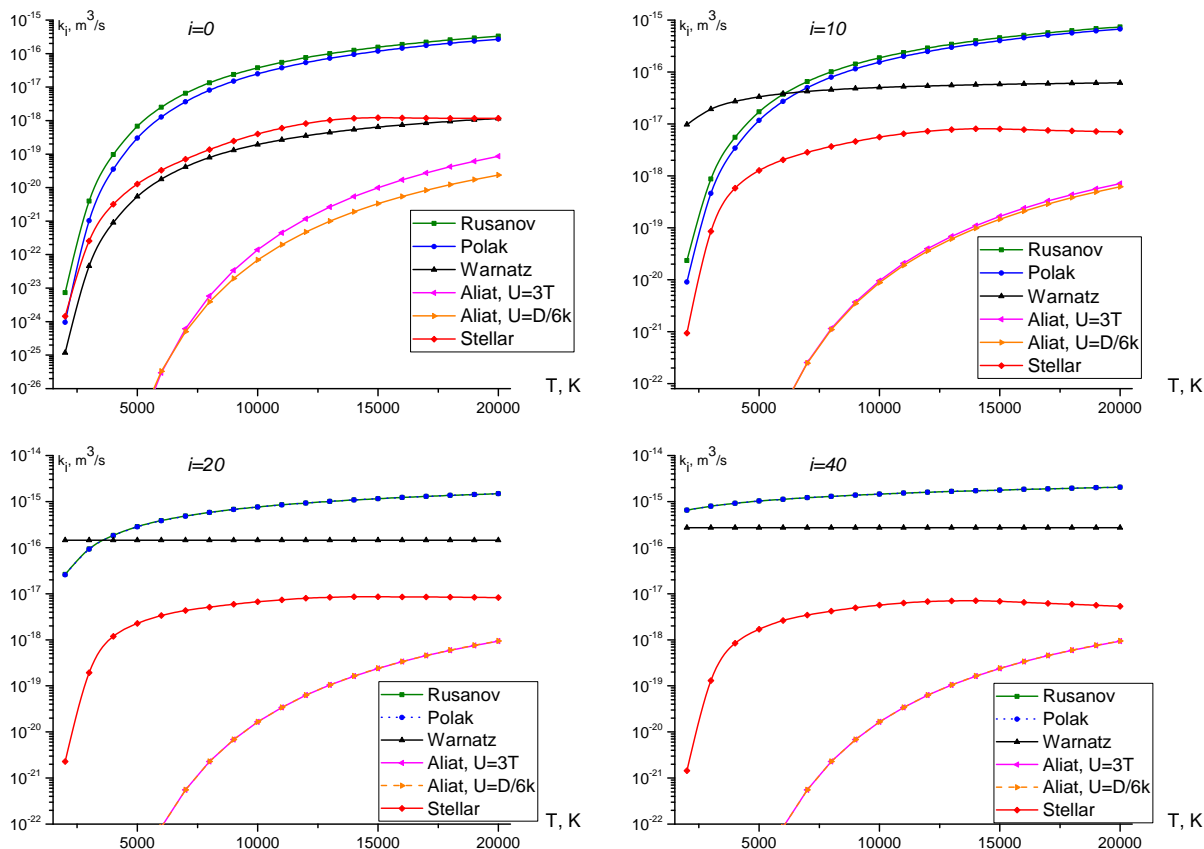


Figure 2: Exchange reaction rate coefficients for  $N_2+O$  reaction as functions of the temperature with fixed  $N_2$  vibrational level for different models.

same time, the coefficients from the Stellar database show a tendency to some decrease in the values with increasing vibrational energy after reaching a certain maximum value. One can notice that for low temperatures, the models of Rusanov-Fridman, Polak, and Warnatz demonstrate fairly close agreement with the Stellar data, whereas the results obtained using the Aliat model are lower by 10–12 orders of magnitude.

With increasing temperature, the picture undergoes qualitative changes: the results of calculations based on the Rusanov-Fridman and Polak models strongly overestimate the exchange reactions rate coefficients as compared to the QCT data, whereas the results based on the Warnatz model continue showing good agreement with the QCT data for the low energy states, but they accumulate the error with increasing the vibrational energy, although less than the first two models. An interesting point is that the results of calculations based on the Aliat model demonstrate a gradual qualitative improvement with increasing temperature and at 20,000 K they give the smallest error among all the considered models in comparison with the QCT data from Stellar.

A similar situation can be observed while comparing the results for the selected levels (Fig. 2). For the 0-th vibrational level, in the entire temperature range the Warnatz model provides the best match with the QCT data, whereas the Rusanov-Fridman and Polak models are not much inferior, and the Aliat model is quite poor at low temperatures. With increasing the energy level, the temperature range where the Rusanov-Fridman and Polak models show the results close to the QCT data is reducing.

As one can see, in the whole range of parameters, the results obtained in the frame of the Rusanov-Fridman and Polak models are very close. Hereafter to simplify the analysis, we keep only the Polak model while comparing the rate coefficients.

It is worth noting that we expected much better results from using the Aliat model and were rather disappointed by the obtained discrepancy. For this reason, we decided to check the formulae and following the methodology proposed in the paper by Aliat<sup>1</sup> we thoroughly re-derived the expressions for the rate coefficients starting from the original Treanor-Marrone model. As a result, the next expression was obtained for the normalizing factor  $C(T, U)$  instead of

the expression (7):

$$C(T, U) = \left[ \sum_{i(1)} \frac{1}{Z_c^{vibr}(T)} \exp\left(-\frac{E_a - \varepsilon_i^c}{kU}\right) + \sum_{i(2)} \frac{1}{Z_c^{vibr}(T)} \exp\left(\frac{E_a - \varepsilon_i^c}{kT}\right) \right]^{-1}, \quad (8)$$

The only difference between the original expression (7) and the new one (8) is the absence of a "minus" sign under the exponent in the second sum. After this simple correction, the results based on the Aliat model demonstrate a significant qualitative improvement in behavior and the best match with the QCT data over the entire range of temperature and vibrational levels as we can see in Fig. 3. Therefore we strongly recommend to use the corrected formula (8) while applying the Aliat model for the exchange reaction rate coefficients.

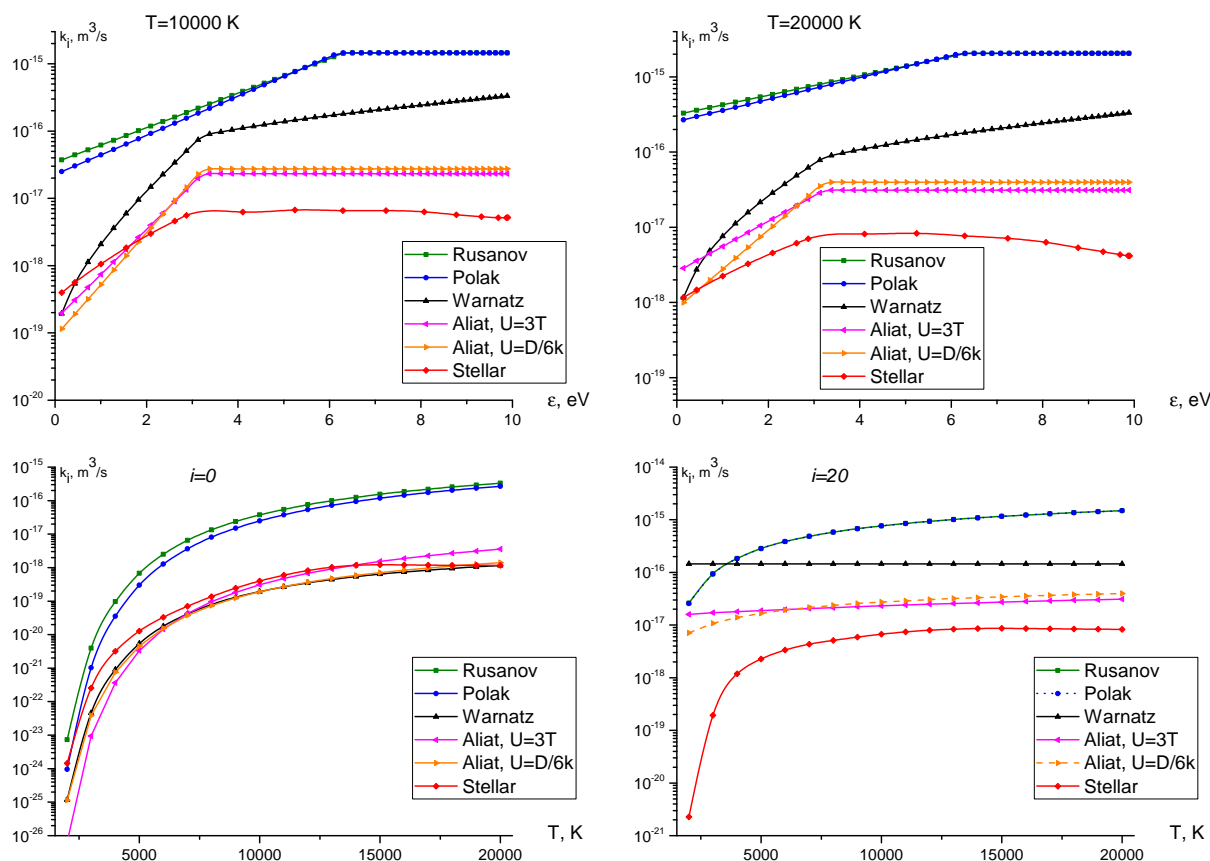


Figure 3: Exchange reaction rate coefficients for  $N_2+O$  reaction for different models with corrected Aliat model.

### 3. Generalization of the Aliat model

As is emphasized in the previous section, all the described theoretical models can be used to calculate the exchange reactions rate coefficients only for the NO ground vibrational energy state,  $k = 0$ . At the same time, the coefficients for all vibrational states of the reaction product are available in the database<sup>15</sup> and also required for the correct state-to-state flow simulations. Based on this arguments we decided to further generalize and improve the model of Aliat. The objective is to introduce some corrections to the original model that would allow us for taking into account not only the vibrational state of the reacting molecule, but also the vibrational state of the reaction product. For carrying out such a refinement, reliable reference data are needed. Until recently, the only source of such data available to us was the data from Stellar.<sup>15</sup> Recently, our colleagues from the NANOTEC CNR (Bari)<sup>4</sup> shared with us their last results on the QCT calculations for the exchange reaction (1) rate coefficients depending on both  $i$  and  $k$ . Then the first step for us was to compare the new data with those from the Stellar database. The results of the comparison are shown in the Fig. 4.

One can see that the general qualitative character of the coefficients dependence on the NO vibrational level is practically the same for both models. Discrepancies are observed only in the absolute values and values for the high-energy states. However the key points are almost identical. This fundamental agreement between the QCT results of

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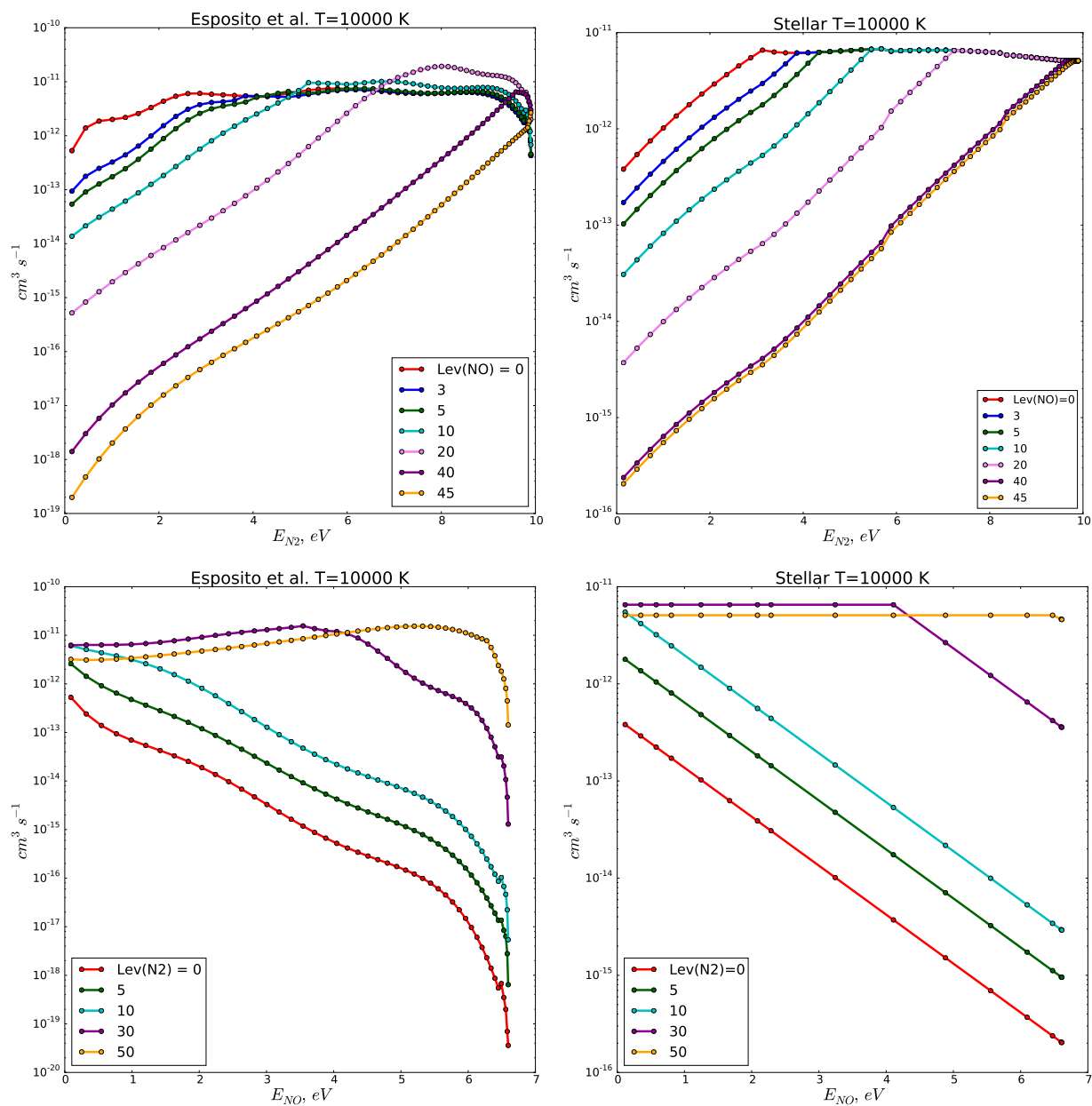


Figure 4: State-specific exchange reaction rate coefficients in  $N_2+O$  collision as functions of  $N_2$  and  $NO$  vibrational energy. QCT results of Esposito<sup>4</sup> and from Stellar database.<sup>15</sup>

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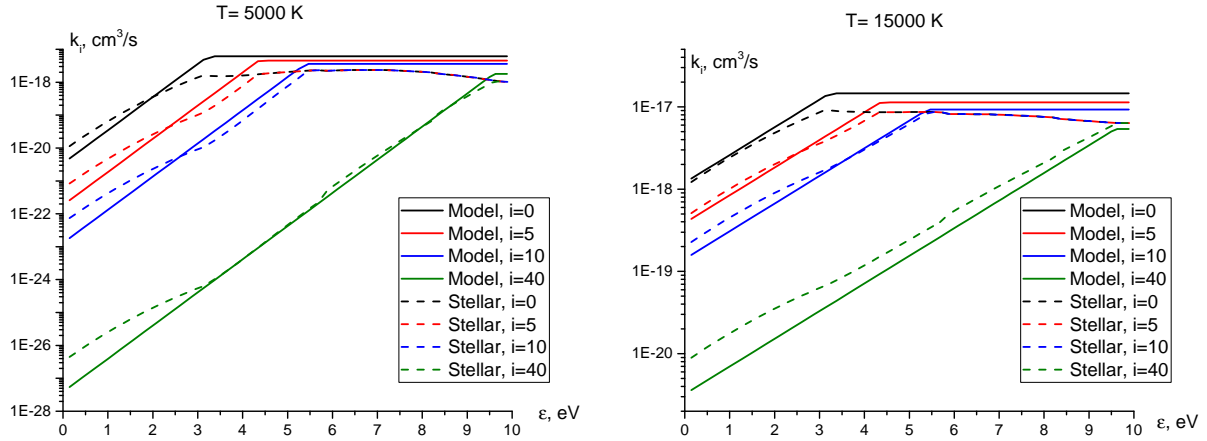


Figure 5: State-specific exchange reaction rate coefficients in  $N_2+O$  collision as functions from  $N_2$  for different NO levels for Stellar and our models.

two independent groups makes it possible to use the results as a base in the construction of the updated model (for further development we use the Stellar data as the reference ones). One of the fundamental facts is the coincidence of points of termination of the coefficients growth for both models. Further analysis shows that this displacement exactly coincides with the energy value of the corresponding vibrational level of the NO molecule. This gives us an idea how to modify the Aliat model: for each selected NO vibrational state we shift the reaction activation energy adding to its value the corresponding NO vibrational energy. The new expression for the rate coefficient takes into account the vibrational level of the reaction product. The updated version written for the reaction (1) is as follows:

$$k_{N_2(i),NO(k)}^{exch}(T, U) = \begin{cases} C(T, U)k_{eq}^{exch} \exp\left(-\frac{E_a + \varepsilon_k^{NO}}{kU}\right) \exp\left[\frac{\varepsilon_i^{N_2}}{k} \left(\frac{1}{T} + \frac{1}{U}\right)\right], & \varepsilon_i^c < E_a + \varepsilon_k^{NO} \\ C(T, U)k_{eq}^{exch} \exp\left(\frac{E_a + \varepsilon_k^{NO}}{kT}\right), & \varepsilon_i^c > E_a + \varepsilon_k^{NO} \end{cases}, \quad (9)$$

$$C(T, U) = \left[ \sum_{i(1)} \frac{1}{Z_{N_2}^{vibr}(T)} \exp\left(-\frac{E_a + \varepsilon_k^{NO} - \varepsilon_i^{N_2}}{kU}\right) + \sum_{i(2)} \frac{1}{Z_{N_2}^{vibr}(T)} \exp\left(\frac{E_a + \varepsilon_k^{NO} - \varepsilon_i^{N_2}}{kT}\right) \right]^{-1}, \quad (10)$$

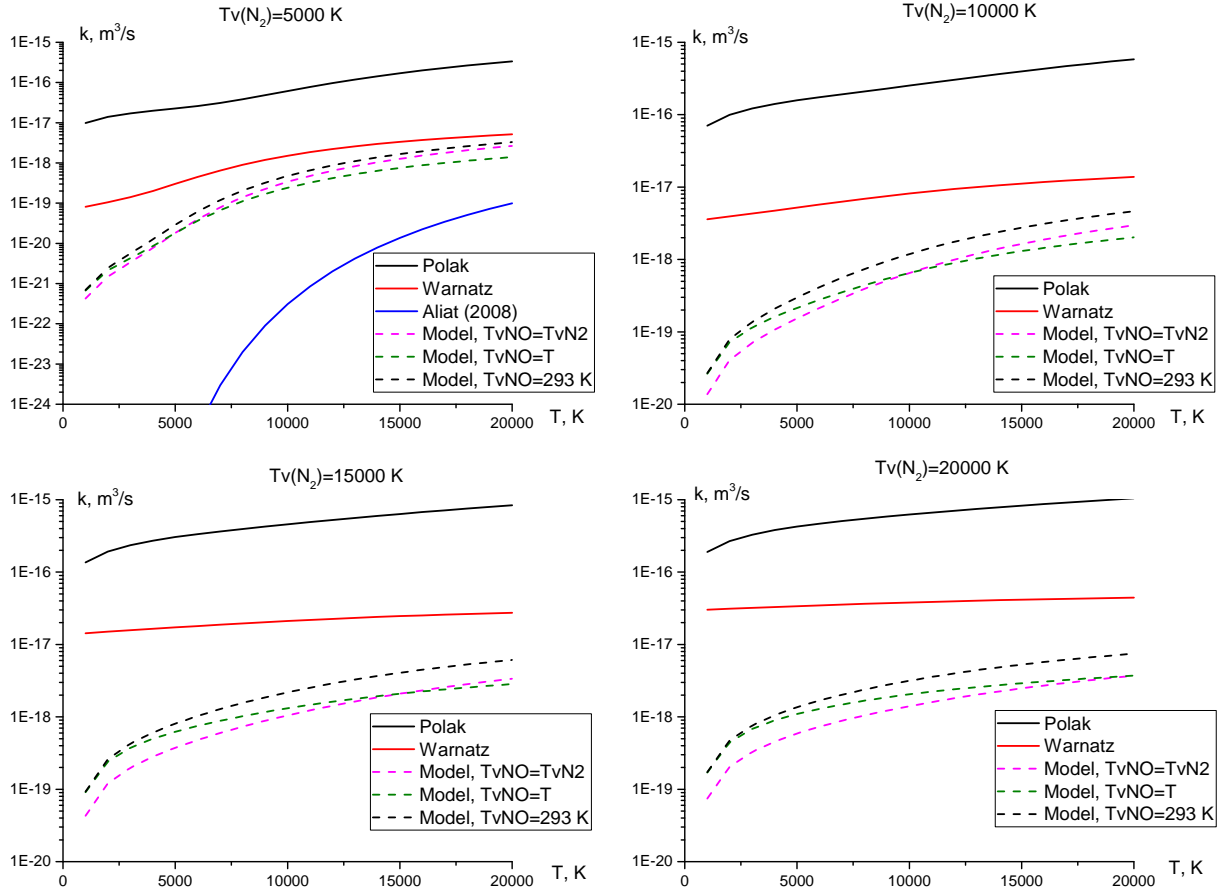
The obtained formula shows a fairly good agreement with the results from the Stellar database in the temperature range from 4000 K to 20000 K. For a better coincidence, the parameters of the Arrhenius law for this reaction also were adjusted. The final recommended values are:  $E_a = 5.175 \cdot 10^{-19}$  J or 3.23 eV,  $A = 0.8 \cdot 10^{-16}$  m<sup>3</sup>/s,  $b = -0.04$ . Thorough comparison of the rate coefficients obtained using our modified model with those from the Stellar database leads to the conclusion that the best fit is achieved for the parameter  $U = \infty$ . The results are shown in Fig. 5. If we compare the results presented in Figs. 3 and 5, we can easily see the following fact: the corrected Aliat model still yields an error up to the one and a half order of magnitude in the entire temperature range and  $N_2$  vibrational levels. At the same time, the generalized model not only reduces this difference by a factor of 5 to 10 for the NO ground energy state, but also ensures the same accuracy for all NO vibrational states over a wide range of temperatures. The most significant discrepancies are observed for the low  $N_2$  levels, which requires some additional investigation, as well as further comparisons with the results of Esposito et al.<sup>4</sup>

Finally, we can see that the new model provides a very good agreement with the data presented by QCT calculations in a wide range of temperature and vibrational states of both  $N_2$  and NO molecules. At the same time, it keeps the simplicity of the original Treanor–Marrone model and thus can be easily implemented to the CFD simulations of high-temperature flows.

#### 4. Multi-temperature rate coefficients

Let us discuss now the multi-temperature reaction rate coefficients. Once the state-to-state reaction rate coefficients are specified, one can easily calculate the averaged rate coefficients using any quasi-stationary vibrational distribution. For the state-resolved models independent of the vibrational state of NO molecules, the averaging is carried out only over

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Figure 6: Two-temperature exchange reaction rate coefficients in  $N_2+O$  collision for different models and temperatures.

the vibrational states of  $N_2$ :

$$k^{exch}(T, T_v^{N_2}) = \frac{1}{n_{N_2}} \sum_i n_i^{N_2}(T_v^{N_2}) k_{N_2(i)}^{exch}(T), \quad (11)$$

where  $n_i^c$  is the number density of molecules  $c$  on the vibrational level  $i$ ,  $n_c = \sum_i n_i^c$  is the number density of  $c$  molecules,  $T_v^c$  is the vibrational temperature of the molecular species  $c$ . For the present study, we use the Boltzmann distributions over vibrational energy.

It is clear that the above expression does not take into account possible NO formation with the temperature different from both gas temperature  $T$  and  $N_2$  vibrational temperature  $T_v^{N_2}$ . Our modified model overcomes this deficiency. While using the rate coefficients (9), one has to make averaging twice, for both  $N_2$  and NO vibrational distributions:

$$k^{exch}(T, T_v^{N_2}, T_v^{NO}) = \frac{1}{n_{N_2} n_{NO}} \sum_i n_i^{N_2}(T_v^{N_2}) \sum_k n_k^{NO}(T_v^{NO}) k_{N_2(i), NO(k)}^{exch}(T). \quad (12)$$

In this case we have the three-temperature reaction rate coefficient depending on  $T$ ,  $T_v^{N_2}$  and  $T_v^{NO}$ . This expression is in the full compliance with the general kinetic-theory model of multi-temperature reacting flows.<sup>10</sup>

The results of calculations of the multi-temperature exchange reaction rate coefficients for different models are shown in the Fig. 6. For the new model developed in the previous section, the results are presented for different NO vibrational temperatures. To analyze the effect of the NO vibrational temperature on the results, we performed two-temperature exchange reaction rate coefficients calculations with three different values of the vibrational temperature of nitrogen oxide:  $T_v^{NO} = T_v^{N_2}$ ,  $T_v^{NO} = T$  and  $T_v^{NO} = 293$  K. The latter case,  $T_v^{NO} = 293$  K is practically equivalent to assuming NO molecules being in the ground state. While taking into account the vibrational excitation of the reaction product leads to the variation in the rate coefficients within one order of magnitude, the use of the Polak and Warnatz models leads to overpredicted values of the rate coefficients by 2–3 orders of magnitude.

Thus we conclude that the choice of the model has a more significant effect on the multi-temperature exchange reaction rate coefficients than the variation of the vibrational temperature of the reaction product. It is worth noting that



in many CFD simulations NO is supposed to be produced either at thermal equilibrium or in the ground vibrational state. Based on the above analysis we can infer that both these assumptions can be applied in simulations of non-equilibrium high-temperature flows without significant loss of accuracy.

## 5. Conclusions

Existing state-resolved theoretical models of the Zeldovich exchange reaction rate coefficients are assessed using the QCT calculations. The discrepancies between quasi-classical trajectory and theoretical models are clearly demonstrated. An error has been discovered and corrected in the original Aliat model; the corrected expressions provide much better agreement with the QCT data than other theoretical models. Generalization of the corrected Aliat model is proposed allowing to take into account the vibrational level of the reaction product. With the optimal choice of the Arrhenius law parameters and the Aliat model parameter, the theoretical state-specific rate coefficients are very close to the QCT ones. The resulting model is quite simple and accurate and can be easily implemented to CFD solvers. On the basis of the state-specific rate coefficients the multi-temperature exchange reaction rate coefficients are calculated as functions of the gas temperature and vibrational temperatures of both reagents and products. The variation of the NO vibrational temperature does not affect significantly the rate coefficients. Therefore the common assumptions that NO molecules are formed either in thermal equilibrium or in the ground state can be used for multi-temperature simulations of non-equilibrium high-temperature flows.

## 6. Acknowledgments

This study is supported by the Russian Science Foundation (project 15-19-30016). The authors are grateful to Maria Nabokova, master student at St. Petersburg State University for her work on data processing of the QCT results and help in the plots preparation.

## References

- [1] A. Aliat. State-to-state dissociation–recombination and chemical exchange rate coefficients in excited diatomic gas flows. *Physica A*, 387:4163–4182, 2008.
- [2] I. Armenise, F. Esposito, and M. Capitelli. Dissociation-recombination models in hypersonic boundary layer flows. *Chem. Phys.*, 336(1):83–90, 2007.
- [3] D. Bose and G.V. Candler. Thermal rate constants of the  $N_2+O \rightarrow NO+N$  reaction using *ab initio*  $^3A''$  and  $^3A'$  potential energy surfaces. *J. Chem. Phys.*, 104(8):2825, 1996.
- [4] F. Esposito and I. Armenise. Reactive, inelastic and dissociation processes in collisions of atomic oxygen with molecular nitrogen. Manuscript submitted, 2017.
- [5] F. Esposito, I. Armenise, and M. Capitelli. N-N<sub>2</sub> state to state vibrational-relaxation and dissociation rates based on quasiclassical calculations. *Chem. Phys.*, 331(1):1–8, 2006.
- [6] F. Esposito, I. Armenise, G. Capitta, and M. Capitelli. O-O<sub>2</sub> state-to-state vibrational relaxation and dissociation rates based on quasiclassical calculations. *Chem. Phys.*, 351(1–3):91–98, 2008.
- [7] O. Kunova, E. Kustova, and A. Savelev. Generalized Treanor–Marrone model for state-specific dissociation rate coefficients. *Chem. Phys. Lett.*, 659:80–87, 2016.
- [8] E. Kustova, E. Nagnibeda, G. Oblapenko, A. Savelev, and I. Sharafutdinov. Advanced models for vibrational-chemical coupling in multi-temperature flows. *Chem. Phys.*, 464:1–13, 2016.
- [9] P.V. Marrone and C.E. Treanor. Chemical relaxation with preferential dissociation from excited vibrational levels. *Phys. Fluids*, 6(9):1215–1221, 1963.
- [10] E.A. Nagnibeda and E.V. Kustova. *Nonequilibrium Reacting Gas Flows. Kinetic Theory of Transport and Relaxation Processes*. Springer-Verlag, Berlin, Heidelberg, 2009.
- [11] Planetary entry integrated models. <http://phys4entrydb.ba.imip.cnr.it/Phys4EntryDB/>.
- [12] L. Polak, M. Goldenberg, and A. Levitskii. *Numerical Methods in Chemical Kinetics*. Nauka, Moscow, 1984. (in Russian).

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- [13] V. Rusanov and A. Fridman. *Physics of Chemically Active Plasma*. Nauka, Moscow, 1984. (in Russian).
- [14] A. S. Savel'ev and E.V. Kustova. Limits of applicability of the Treanor-Marrone model for  $N_2$  and  $O_2$  state-to-state dissociation rate coefficients. *Vestnik of Saint Petersburg University. Series I. Mathematics. Mechanics. Astronomy*, 2 (60)(2):268–279, 2015.
- [15] Stellar database. <http://esther.ist.utl.pt/pages/stellar.html>.
- [16] J.B. Warnatz, U. Riedel, and R. Schmidt. Different levels of air dissociation chemistry and its coupling with flow models. In *Advances in Hypersonics: Modeling Hypersonic Flows*. Birkhäuser, Boston, 1992.