



Advanced models for vibrational–chemical coupling in multi-temperature flows



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ABSTRACT

In this paper, self-consistent models for coupled vibrational relaxation and dissociation in multi-temperature gas mixture flows are proposed on the basis of the kinetic theory methods. The Treanor–Marrone dissociation model is generalized taking into account the dependence of model parameter on the vibrational state. Multi-temperature dissociation rate coefficients are calculated on the basis of the improved Treanor–Marrone model using the Boltzmann and Treanor vibrational distributions; comparison with traditional models shows a significant difference in the dissociation rate coefficients for high temperatures. Generalization of the well known Landau–Teller model overcoming limitations of the original model is proposed. The developed models are validated against experimental data and assessed in non-equilibrium shock heated flows of O_2/O and N_2/N mixtures. It is shown that the proposed models provide a good accuracy in the wide range of flow conditions while being simple and computationally efficient.

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1. Introduction

Modeling of thermochemically non-equilibrium flows remains a challenging problem of hypersonic aerothermodynamics during the last decades. Although a wide variety of models for vibrational relaxation and chemical reactions have been proposed, the accuracy of fluid dynamic variables and heat transfer predictions still requires assessment and improvement.

The most detailed description of strongly non-equilibrium reacting gas flows in the frame of continuum media approach is given by the state-to-state model [1–3]. This model treats each vibrational (or rovibrational) state of a molecule as a separate chemical species. Solving the master equations coupled to the fluid dynamic equations one can find the flow-field and the populations of internal states. The main advantage of the state-to-state approach is that it does not adopt any quasi-stationary distribution over internal energy states and therefore can be applied for arbitrary deviations from thermochemical equilibrium. This model is widely used now for simulations of stationary 1D [4–12] and simple 2D [13–15] flows. However its implementation for modeling complex 2D and 3D problems is hardly feasible due to very high computational costs, especially for viscous flow simulations requiring calculations of the state-to-state transport properties [16,17]. To the authors' knowledge, 3D simulations using the

state-to-state approach have been done only in [18]. As a consequence, development of reduced multi-temperature models is of importance for engineering applications.

Multi-temperature flow description is based on the assumption that a part of vibrational energy transitions proceeds faster than vibration–translation (VT) exchange and chemical reactions. Fast vibration–vibration (VV) transitions result in establishing quasi-stationary distributions over vibrational energy. Commonly used multi-temperature models are based on the Boltzmann vibrational distributions for harmonic oscillators [19,20]; their application is limited to flow conditions with weak impact of anharmonicity. Advanced multi-temperature models have been developed for the Treanor distribution taking into account near-resonant VV exchange [21–23] and for more sophisticated combined Treanor–Gordiets–Boltzmann distribution accounting for different rates of vibrational transitions at various vibrational levels [24–26]. Reduced models based on the analysis of state-to-state distributions are discussed in [27,28]. An interesting model combining several Boltzmann distributions for different parts of the vibrational ladder is proposed recently in [29].

Development of a multi-temperature flow description requires modeling of vibrational relaxation, chemical reactions and coupling of these processes. For the state-dependent rate coefficients of vibrational transitions many models have been proposed, both analytical [30,4,31] and those based on molecular dynamic simulations [32–41]. Nonetheless in the multi-temperature flow simulations the Landau–Teller relaxation equation [42] with the

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Millikan–White relaxation time [43] is still commonly used, sometimes with empirical corrections [20]. It is worth noting that although the original Landau–Teller equation has been derived for weak deviations from thermal equilibrium under assumption of harmonic oscillations, at the present time it is widely implemented into the computational fluid dynamics (CFDs) for strongly non-equilibrium conditions and arbitrary model of vibrational spectra. Recently, a self-consistent model for the rate of vibrational relaxation based on the Chapman–Enskog method has been proposed in the frame of the state-to-state [44] and multi-temperature [45] flow descriptions. It is shown that in viscous flows, the rate of vibrational relaxation is specified by the rates of all other slow processes; the cross-coupling effect between the stress tensor and reaction rates is demonstrated. In the present study we use the model developed in [45] to assess the mixture thermochemical properties and establish the limits of applicability for the Landau–Teller equation.

Rates of chemical reactions are of crucial importance for the accurate prediction of the non-equilibrium flow dynamics and heat transfer. In vibrationally non-equilibrium flows, it is necessary to account for strong coupling of vibrational relaxation and chemistry, and one-temperature Arrhenius rate coefficients are not applicable. There are numerous models of cross-coupling between vibrational and chemical non-equilibrium such as CVDV [46–50] (coupled vibration–dissociation–vibration), CVCV [51,50] (coupled vibration–chemistry–vibration), but they are basically applicable only to inviscid flows (except [49]) and rely on quasi-empirical expressions for the coupling terms derived on the basis of the Boltzmann vibrational distributions. On the other hand, as is demonstrated in [6,8,52,53], the averaged reaction rate coefficients depend strongly on the shape of non-equilibrium distributions. The model developed in [45] overcomes these limitations, however the coupling terms derived in this paper have a rather complicated form and it is hard to implement them directly into 3D viscous flow solvers. Therefore it is interesting to assess simpler models. For this purpose we have chosen the Treanor–Marrone CVDV model. It is quite simple, efficient and is widely used in many hypersonic applications. The model contains an adjustable parameter which is basically set to constant. A thorough analysis performed in [54] showed that setting this parameter to the constant value or linear function of temperature cannot provide satisfactory agreement with dissociation rate coefficients obtained from the molecular dynamic calculations. Accurate definition of the parameter in the Treanor–Marrone model can significantly improve the predicted dissociation rates in non-equilibrium flows.

The objectives of the present paper are:

- To generalize the Treanor–Marrone model taking into account the dependence of its parameter on the vibrational state and temperature.
- To estimate the impact of the model and different vibrational distributions on the multi-temperature dissociation rate coefficients.
- To derive a rigorous model of VT relaxation and establish the limits of applicability for the Landau–Teller model.
- To validate the proposed models.
- To study the shock heated flows of binary mixtures O_2/O and N_2/N .

The paper is organized as follows. First we develop the generalized Treanor–Marrone model and study multi-temperature dissociation rate coefficients. Then we introduce the accurate model for the vibrational–chemical coupling and discuss its relation to the Landau–Teller equation. Then the models are applied to the high-temperature binary mixture flows behind the shock waves. Distribution of fluid dynamic variables in O_2/O and N_2/N mixtures

calculated under various free stream conditions on the basis of modified Treanor–Marrone and Landau–Teller expressions are compared with those found experimentally [55] as well as with the solutions obtained using the traditional models such as original Landau–Teller and Treanor–Marrone models, the forced harmonic oscillator model (FHO) [31], and analytical expressions of Shwartz, Slawsky and Herzfeld (SSH) [30]. The results allow estimating the limits of applicability for the proposed simple and numerically efficient models.

2. Generalized Treanor–Marrone model

Modeling of vibration–dissociation coupling in reacting flows still represents a challenging task. Experimental measurement of dissociation rate coefficients in vibrationally non-equilibrium flows is fairly complicated, and consequently, experimental data on the state-to-state or multi-temperature dissociation rate coefficients are scarce (some recent experimental results for oxygen can be found in [55]). In this situation, molecular dynamic methods are suitable to provide missing information on the reaction cross sections and state-specific rate coefficients [35–40]. However direct implementation of trajectory calculations into hypersonic flow simulations is not feasible at the present time due to extremely high computational efforts. Moreover, the state-to-state dissociation rate coefficients provided in the database [40] are given only for a few selected vibrational states, and the proposed interpolation formulas are valid for the temperatures lower than 10,000 K. Therefore accurate analytical models for vibration–dissociation coupling are of importance for computational fluid dynamics.

Theoretical models for multi-temperature dissociation rate coefficients have been proposed by many authors. The simplest empirical Park’s model widely used in CFD is described in [20]; analytical Treanor–Marrone, Kuznetsov, Macheret–Fridman models [46–48] are better justified but sometimes contain cumbersome expressions hardly implementable to CFD solvers. Theoretical models generally include adjustable parameters, and correct choice of these parameters can significantly improve the model accuracy. For the present study, we have chosen the Treanor–Marrone model of preferential dissociation first proposed for two-temperature flows of harmonic oscillators in [46] and later generalized for multi-temperature flows of anharmonic oscillators [23] and for the state-to-state model [54]. This simple model is based on clear physical reasoning and can be easily applied for non-equilibrium flow simulations. The Treanor–Marrone model involves one adjustable parameter U having the dimension of temperature and characterizing the decrease in the dissociation rate with decreasing in the vibrational level. In CFD, this parameter is basically set to constant, $U = \infty$ (which corresponds to equiprobable dissociation from each vibrational level), $U = D/(6k)$ (D is the dissociation energy, k is the Boltzmann constant), or it is defined as a linear function of temperature, for instance, $U = 3T$. The latter two cases describe preferential dissociation from high vibrational levels. Analysis performed in [54,56] shows that constant values of U (or linear function of T) cannot provide satisfactory agreement of the state-specific dissociation rate coefficients with those obtained by quasi-classical trajectory calculations in the whole range of temperature and vibrational states.

Let us consider first the state-to-state modification of the Treanor–Marrone model. The rate coefficient $k_{i,diss}^M$ of dissociation from the vibrational state i after a collision with a partner M can be calculated in the form:

$$k_{i,diss}^M = Z_i^M k_{diss,eq}^M(T) \quad (1)$$

where $k_{diss,eq}^M(T)$ is the thermal equilibrium dissociation rate coefficient, Z_i^M is the non-equilibrium factor determined as:

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